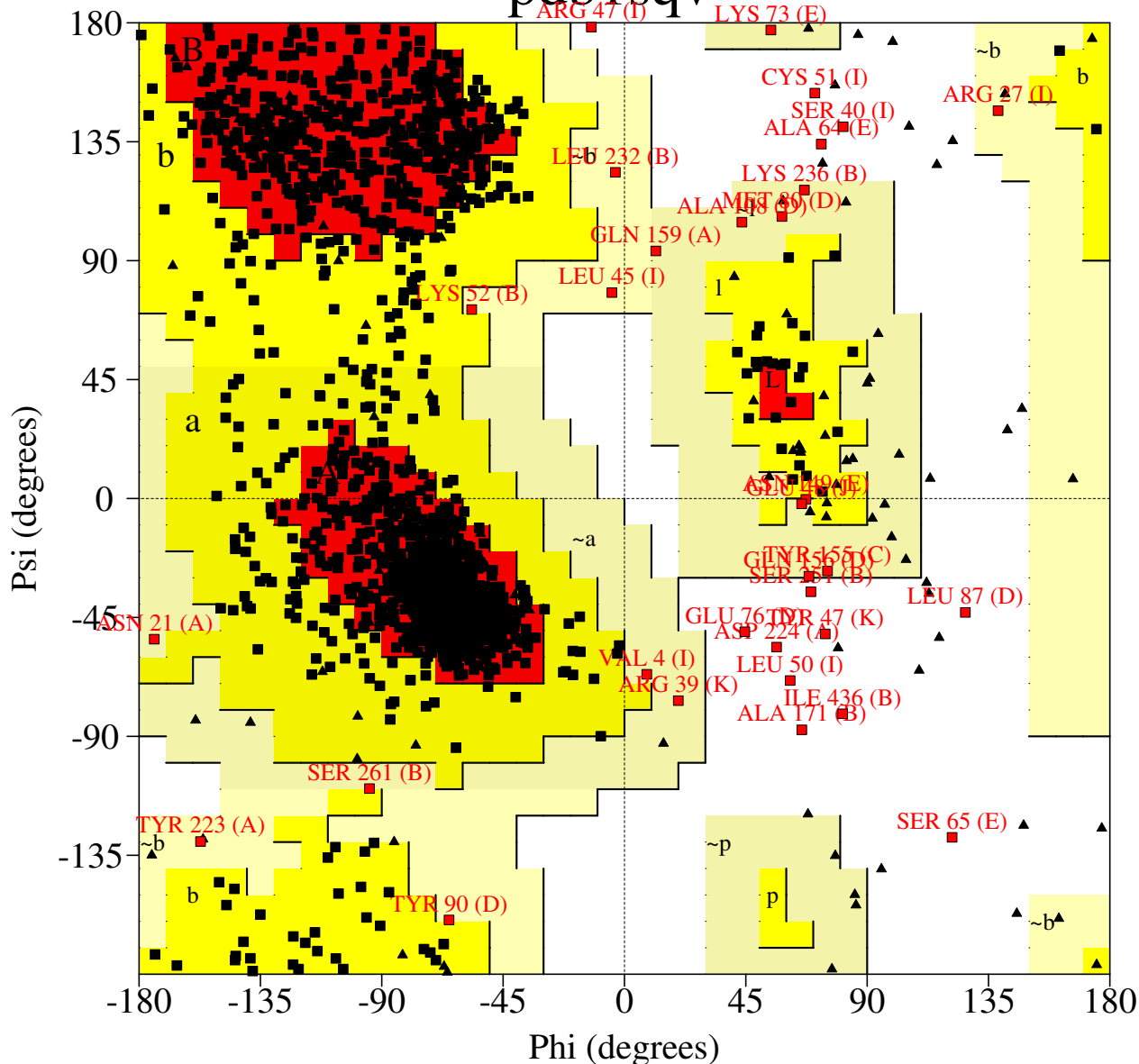


# Ramachandran Plot

pdb1sqv



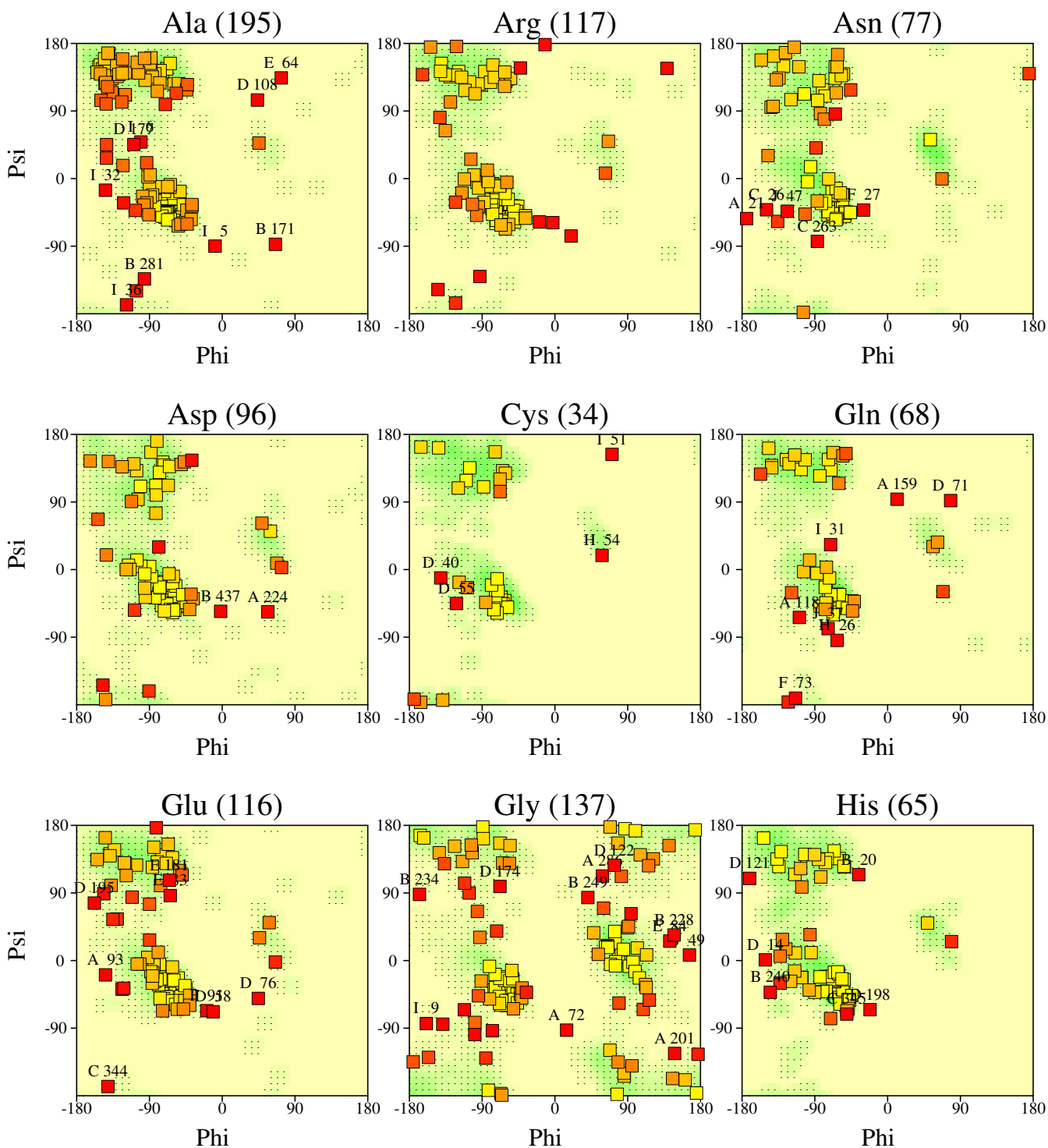
### Plot statistics

Residues in most favoured regions [A,B,L]	1558	85.0%
Residues in additional allowed regions [a,b,l,p]	242	13.2%
Residues in generously allowed regions [-a,-b,-l,-p]	19	1.0%
Residues in disallowed regions	13	0.7%
-----		
Number of non-glycine and non-proline residues	1832	100.0%
Number of end-residues (excl. Gly and Pro)	19	
Number of glycine residues (shown as triangles)	140	
Number of proline residues	109	
-----		
Total number of residues	2100	

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

# Ramachandran plots for all residue types

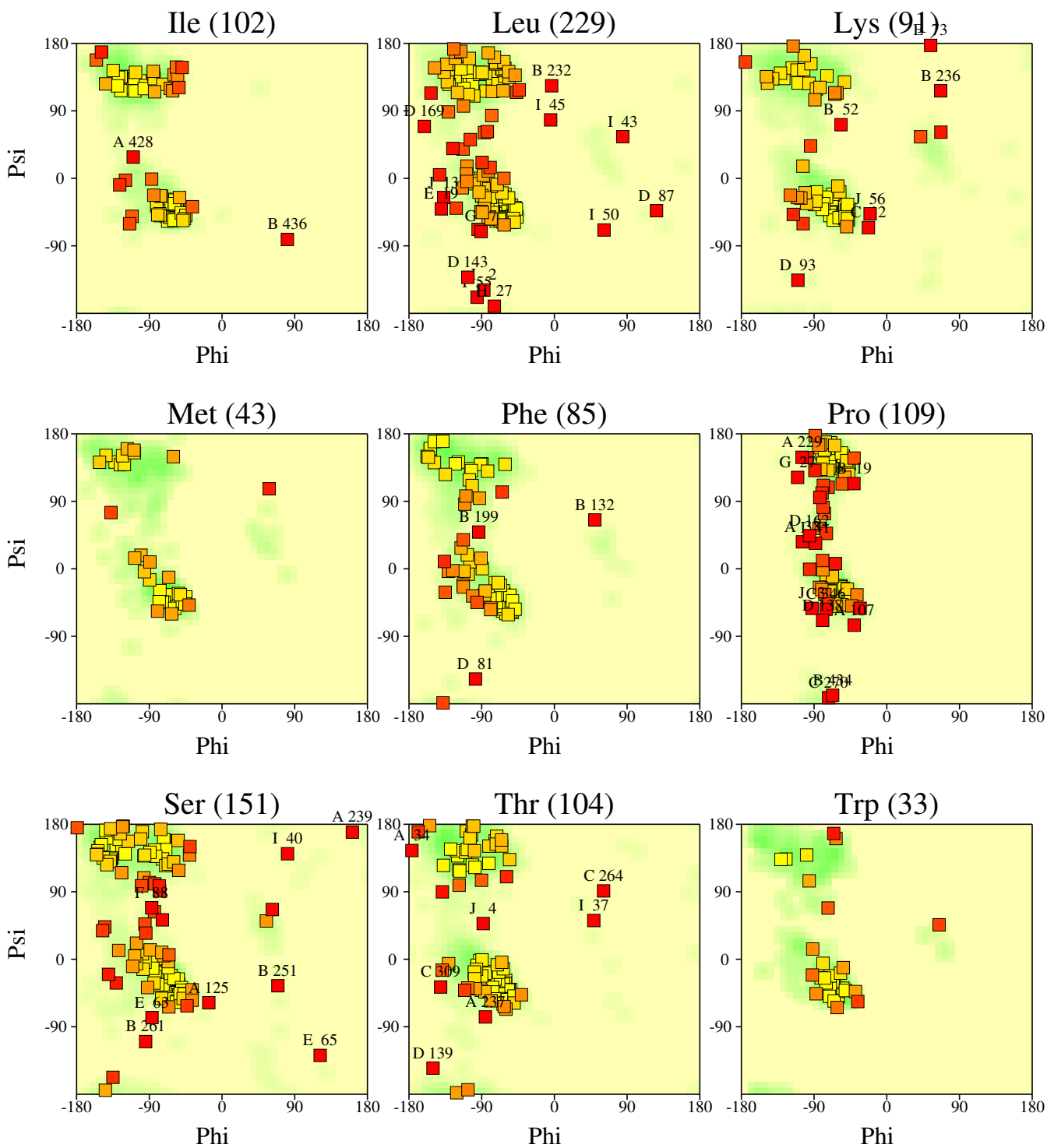
## pdb1sqv



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

# Ramachandran plots for all residue types

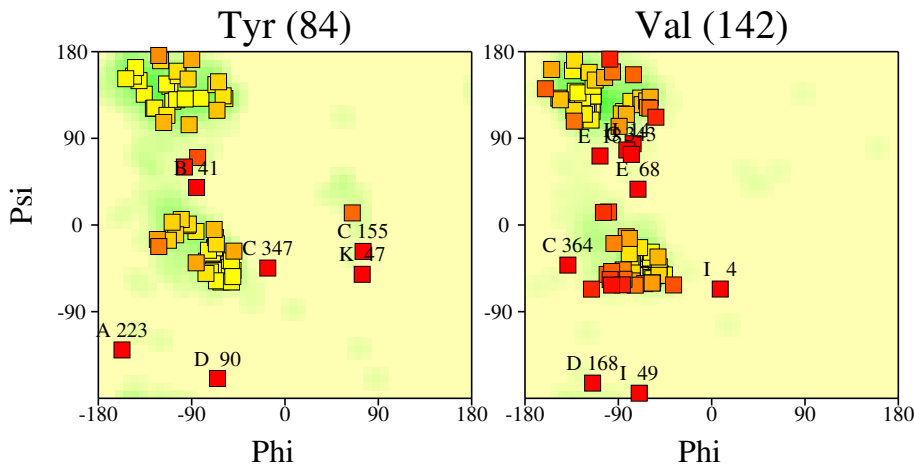
## pdb1sqv



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

# Ramachandran plots for all residue types

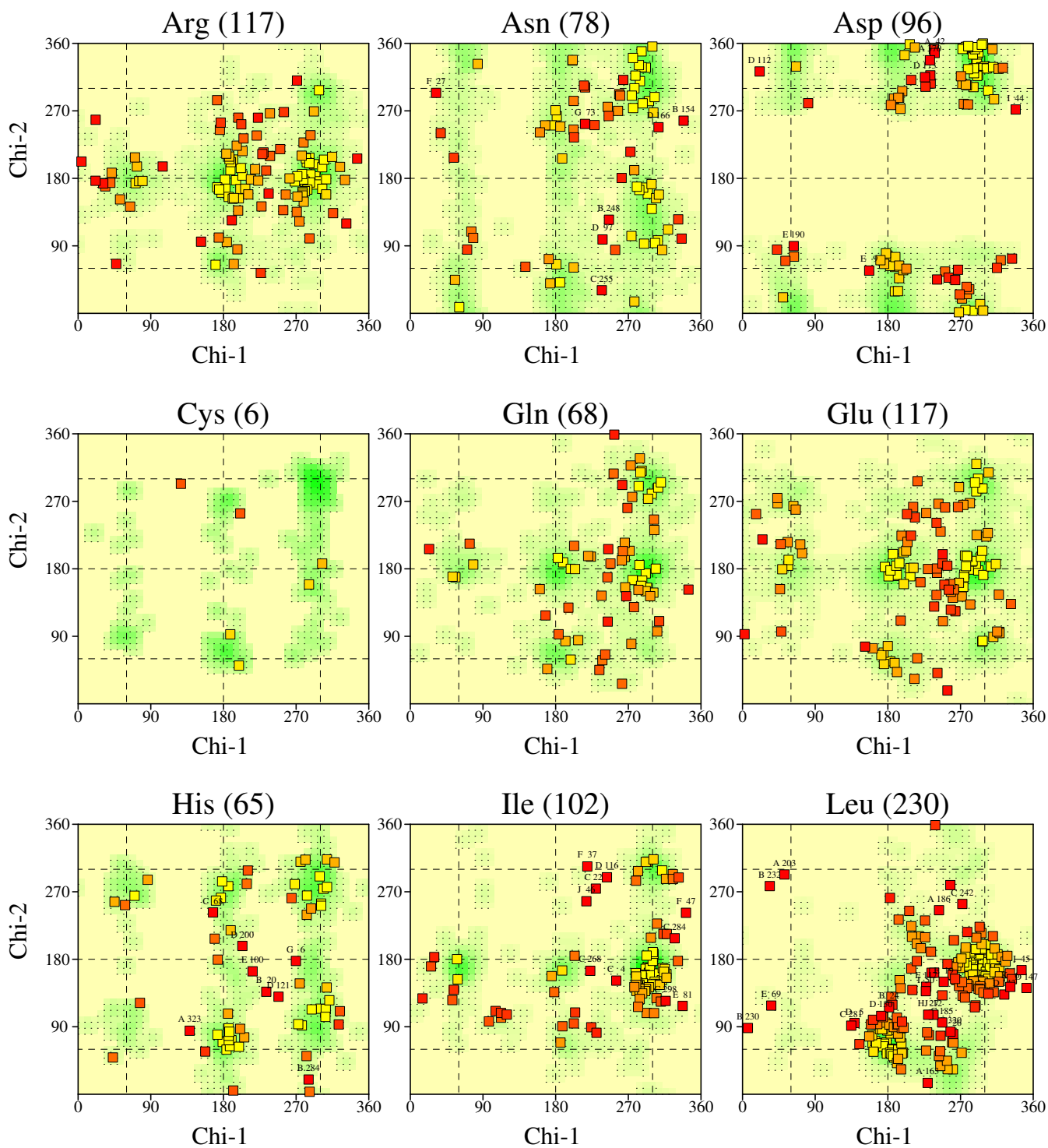
pdb1sqv



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

# Chi1-Chi2 plots

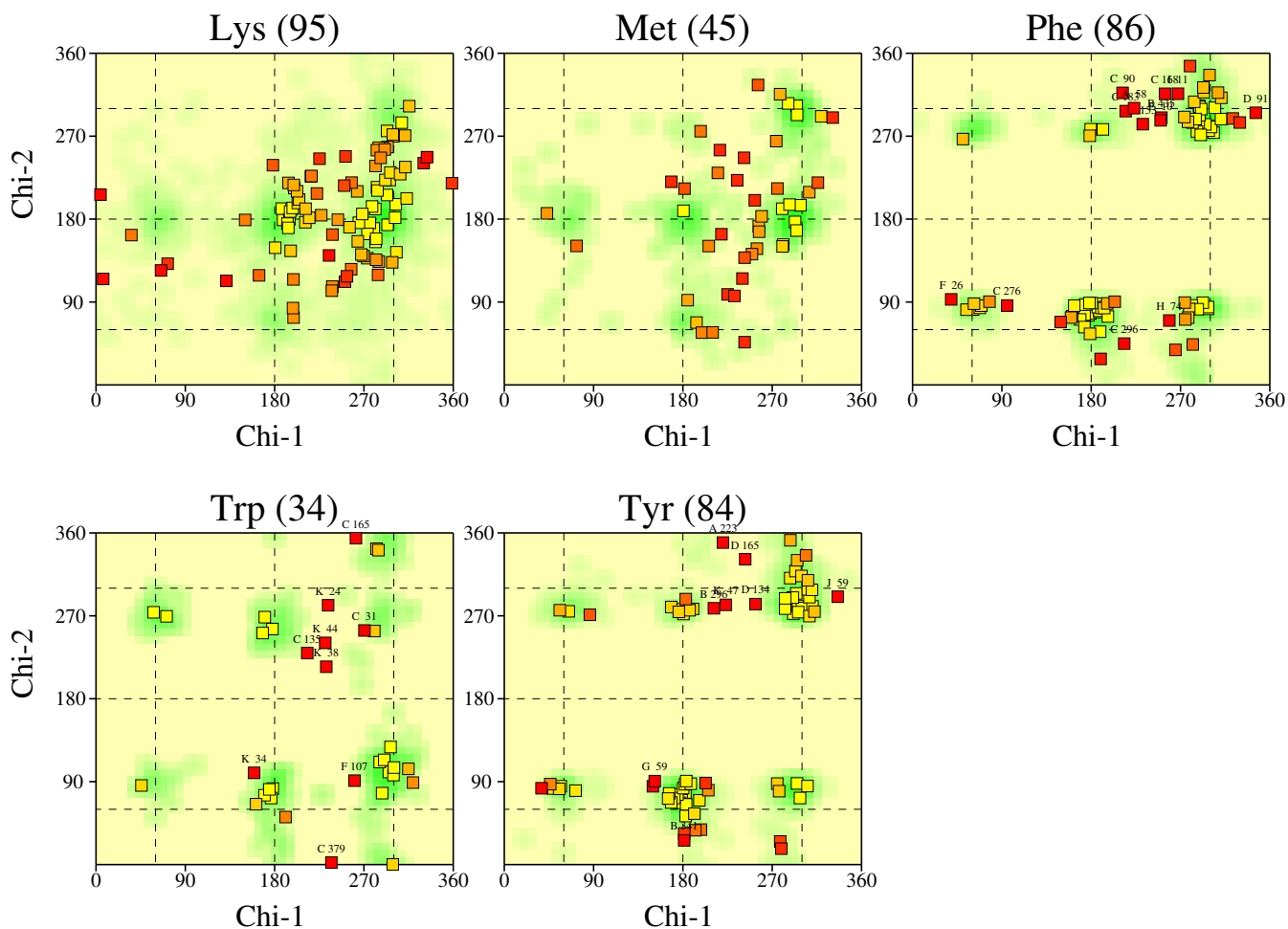
## pdb1sqv



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0Å or better.

# Chi1-Chi2 plots

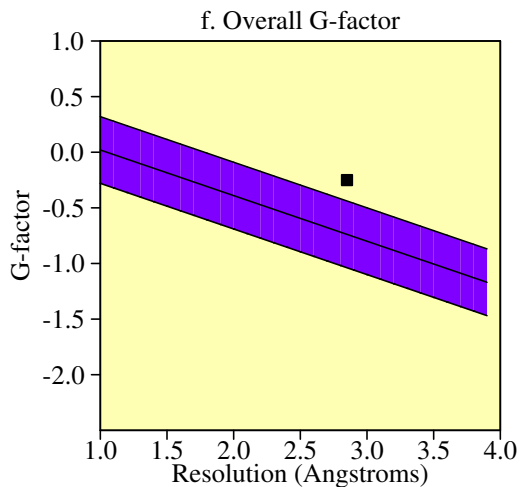
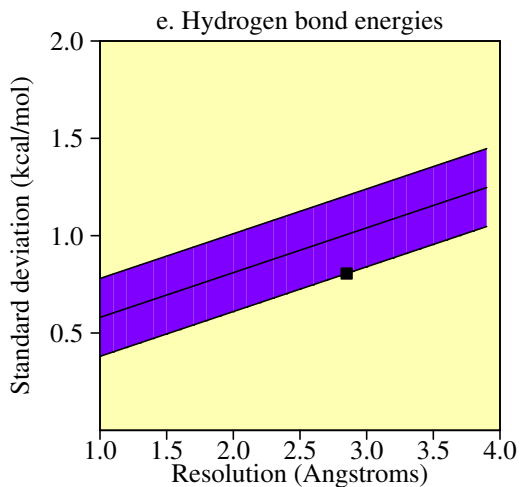
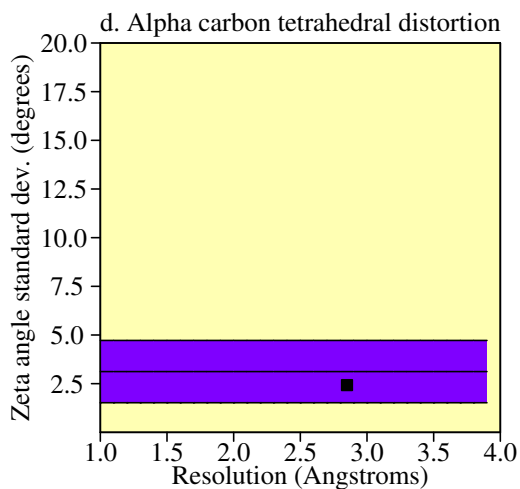
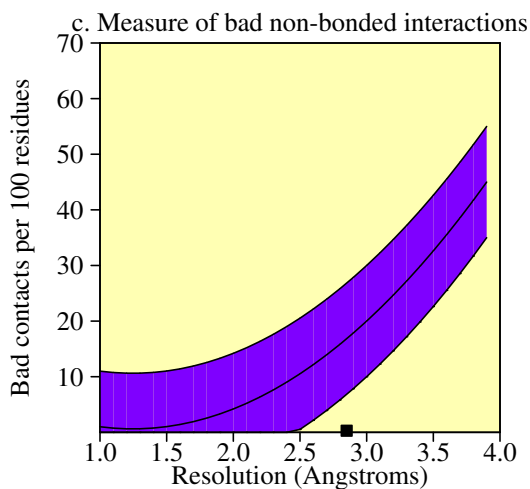
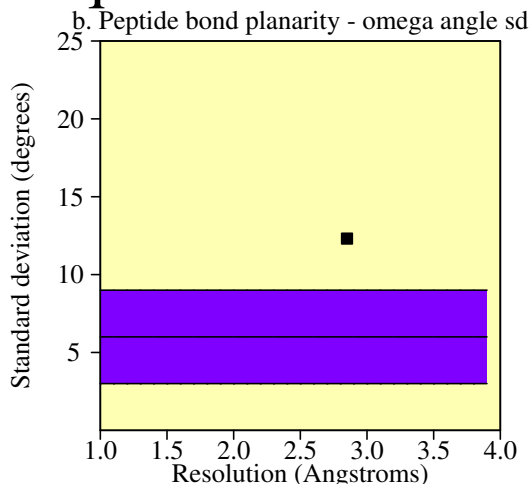
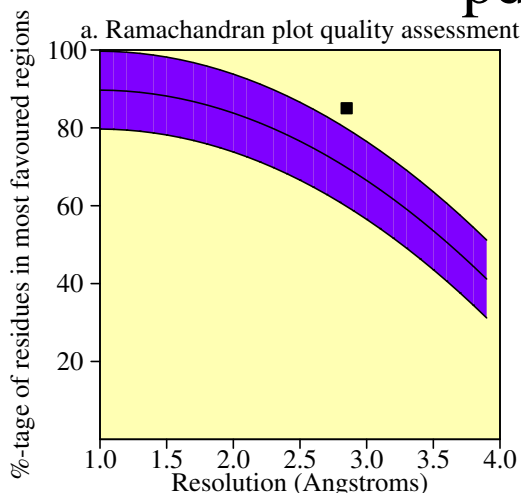
## pdb1sqv



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

# Main-chain parameters

pdb1sqv

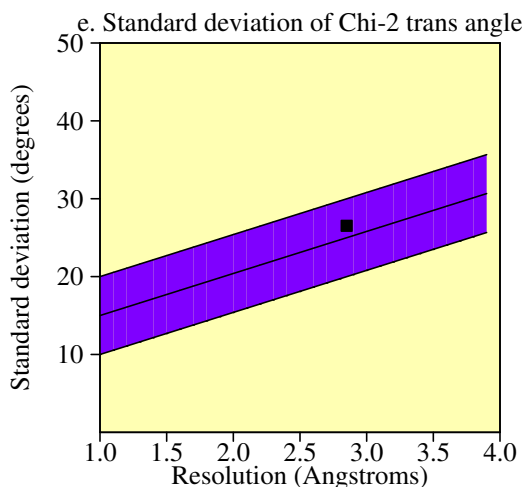
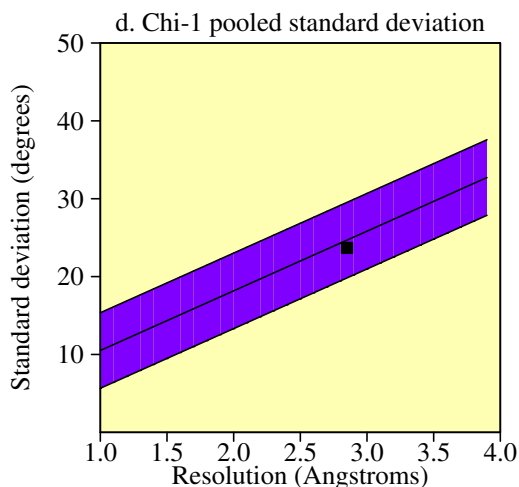
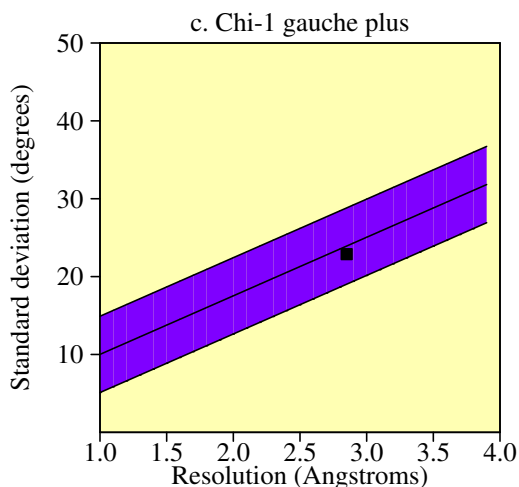
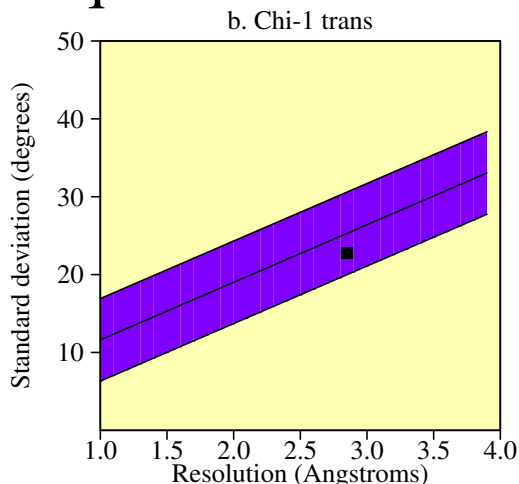
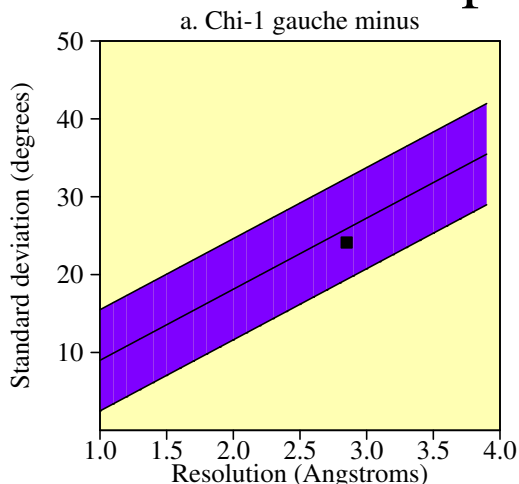


### Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
a. %-tage residues in A, B, L	1832	85.0	69.8	10.0	1.5	BETTER
b. Omega angle st dev	2088	12.3	6.0	3.0	2.1	WORSE
c. Bad contacts / 100 residues	6	0.3	16.8	10.0	-1.7	BETTER
d. Zeta angle st dev	1960	2.4	3.1	1.6	-0.4	Inside
e. H-bond energy st dev	1352	0.8	1.0	0.2	-1.0	Inside
f. Overall G-factor	2100	-0.3	-0.7	0.3	1.6	BETTER

# Side-chain parameters

## pdb1sqv



pdb1sqv

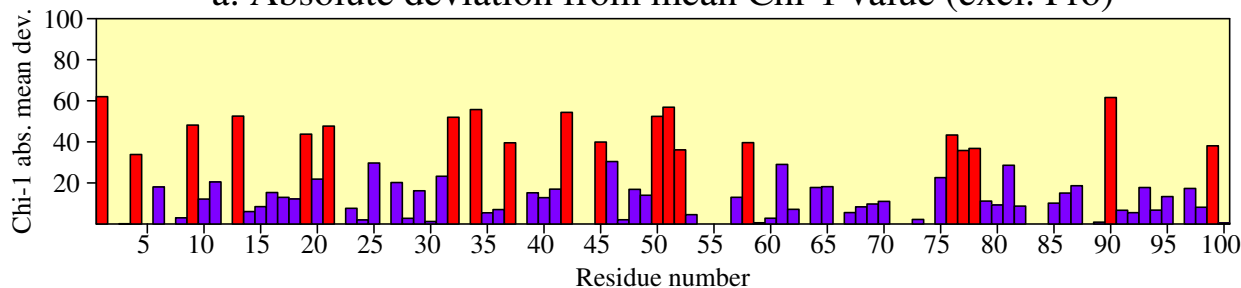
### Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
a. Chi-1 gauche minus st dev	240	24.1	25.9	6.5	-0.3	Inside
b. Chi-1 trans st dev	602	22.8	25.3	5.3	-0.5	Inside
c. Chi-1 gauche plus st dev	813	22.9	23.9	4.9	-0.2	Inside
d. Chi-1 pooled st dev	1655	23.7	24.7	4.8	-0.2	Inside
e. Chi-2 trans st dev	516	26.5	25.0	5.0	0.3	Inside

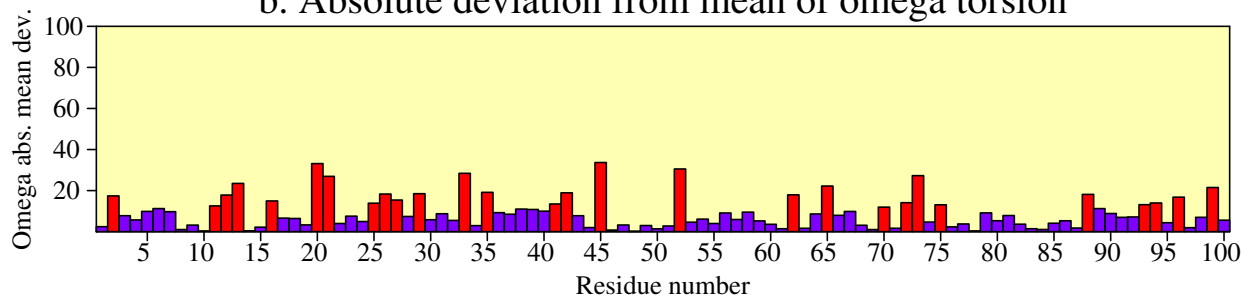


# Residue properties pdb1sqv

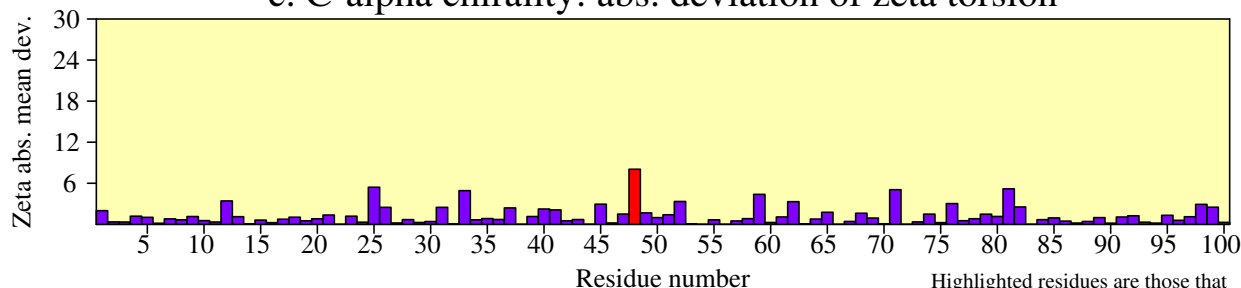
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

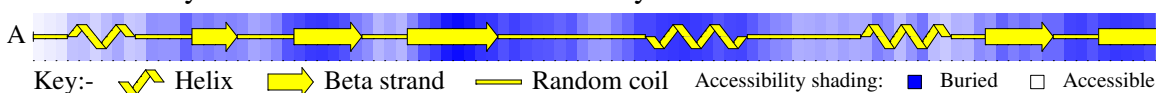


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

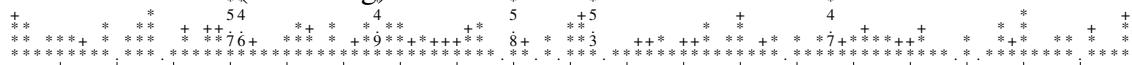
d. Secondary structure & estimated accessibility



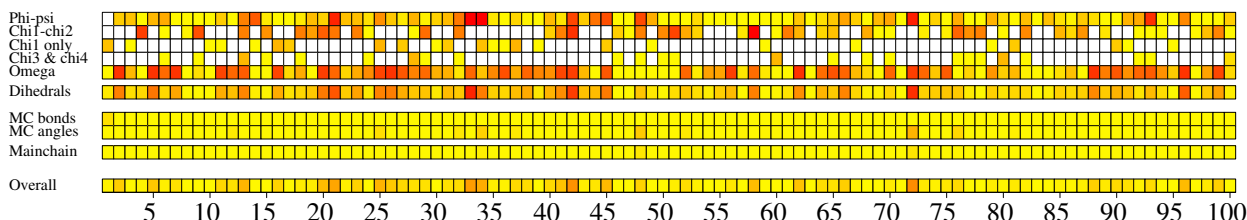
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

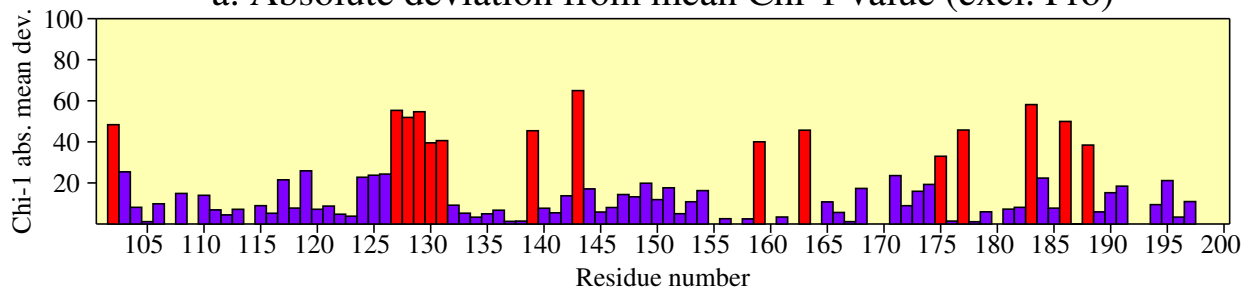


g. G-factors

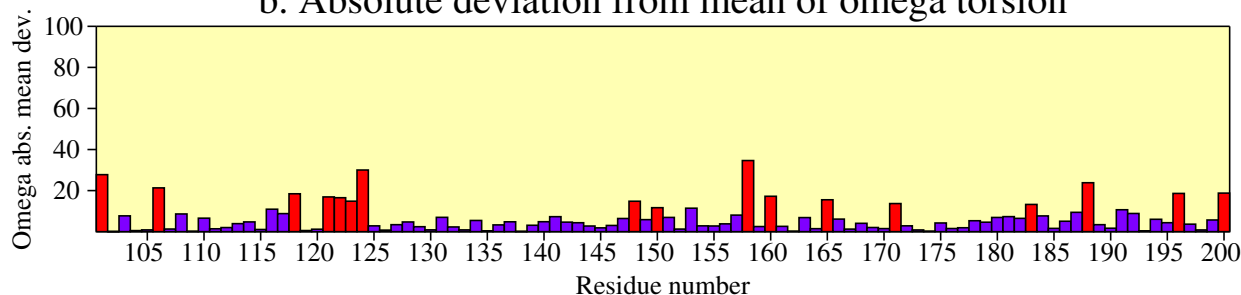


# Residue properties pdb1sqv

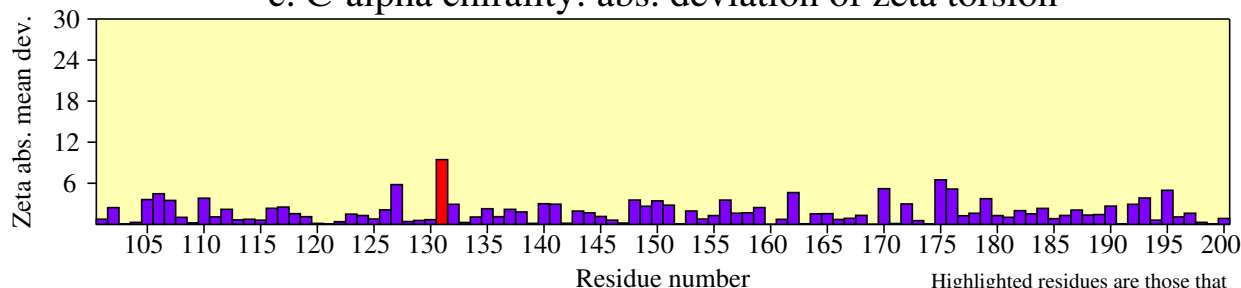
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

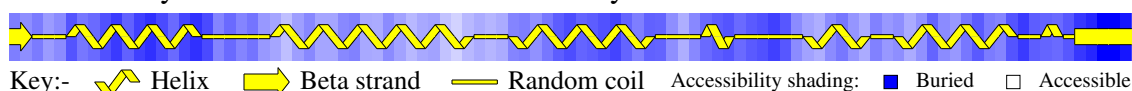


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

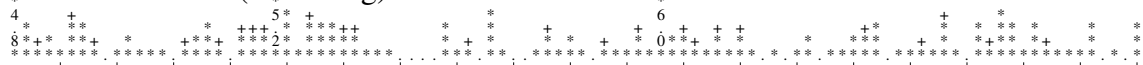
### d. Secondary structure & estimated accessibility



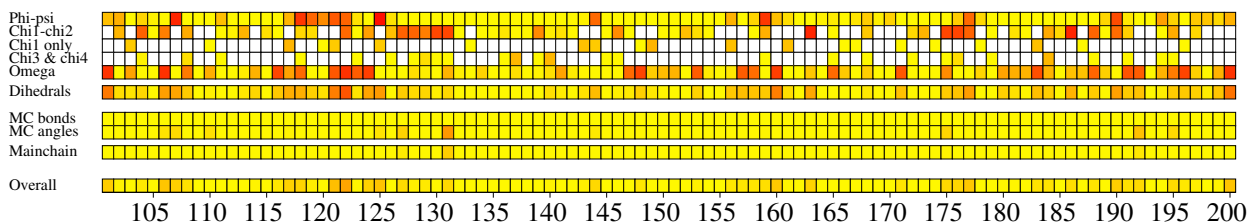
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

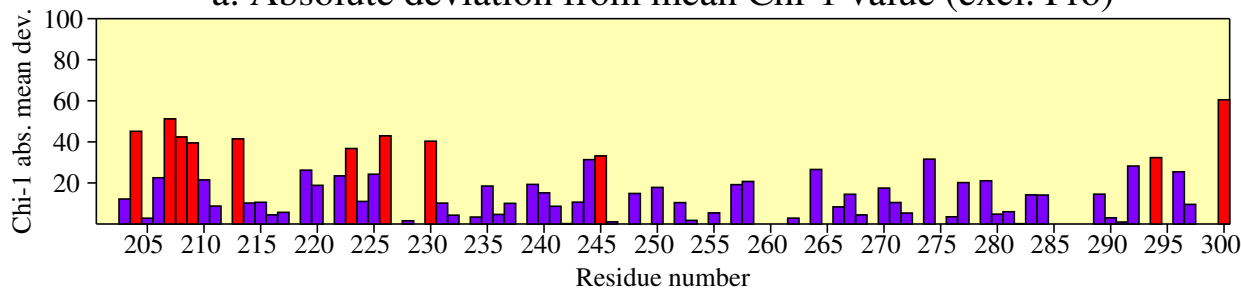


### g. G-factors

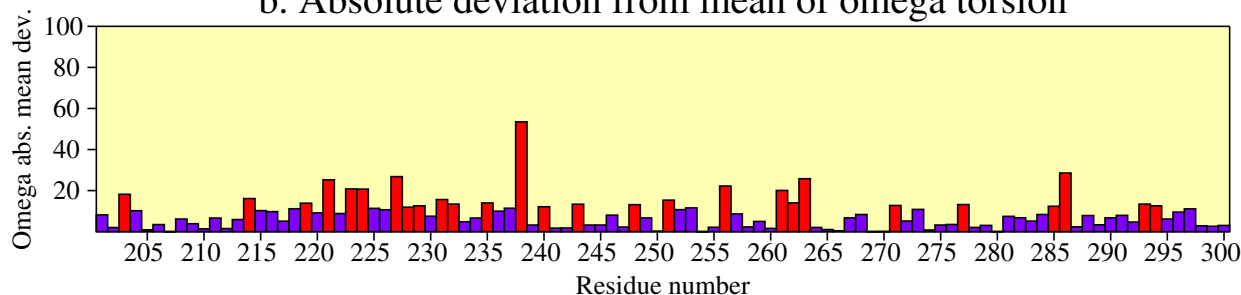


# Residue properties pdb1sqv

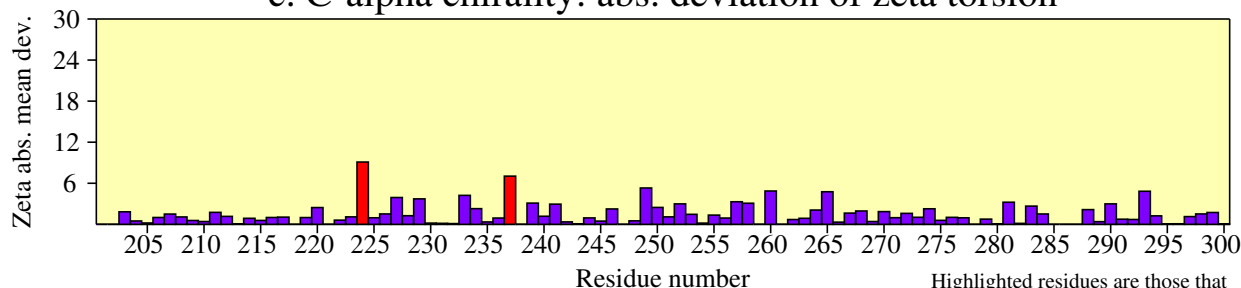
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

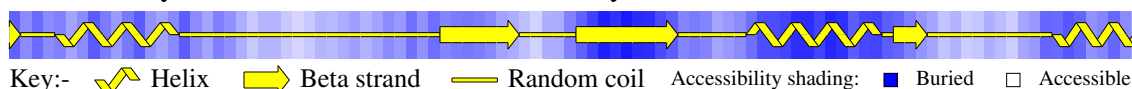


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

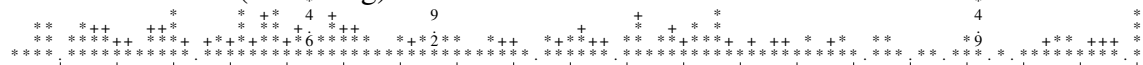
d. Secondary structure & estimated accessibility



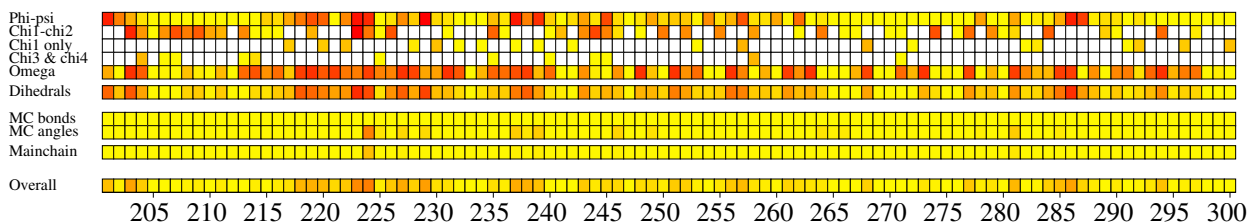
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

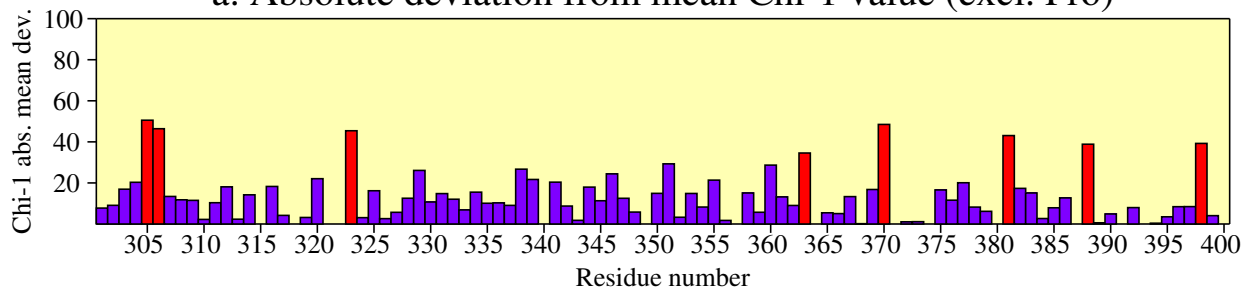


g. G-factors

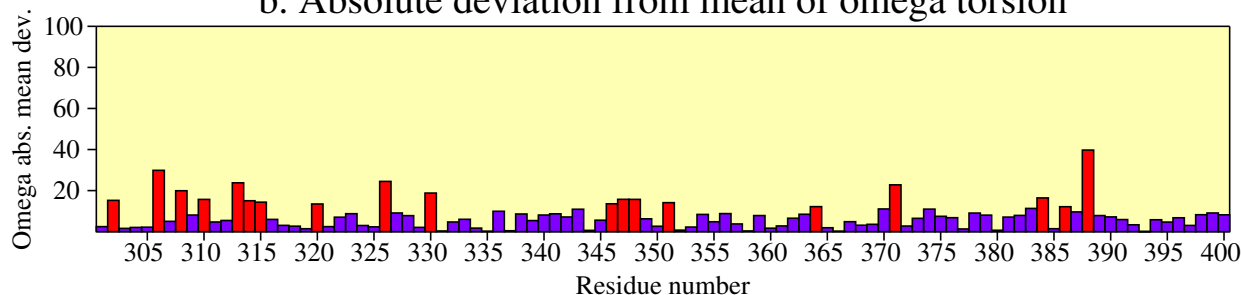


# Residue properties pdb1sqv

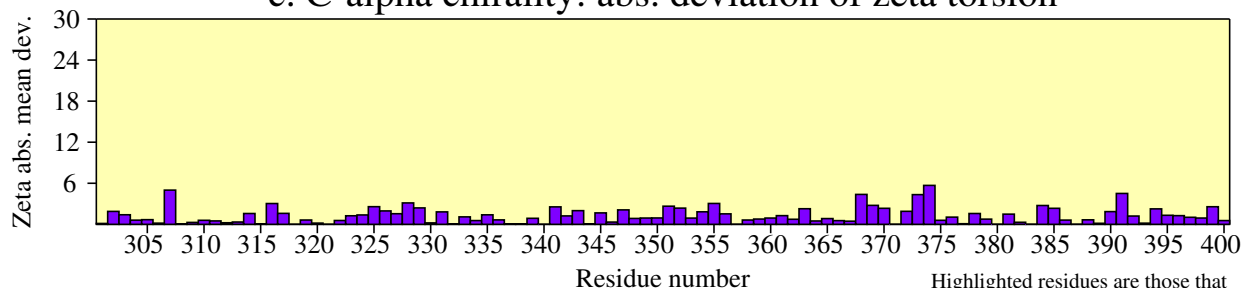
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

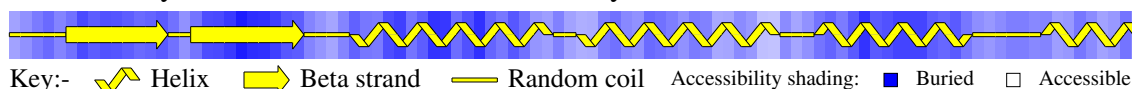


c. C-alpha chirality: abs. deviation of zeta torsion

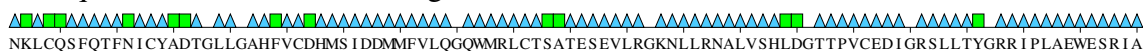


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

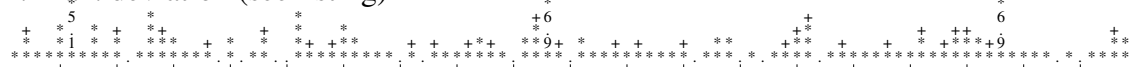
d. Secondary structure & estimated accessibility



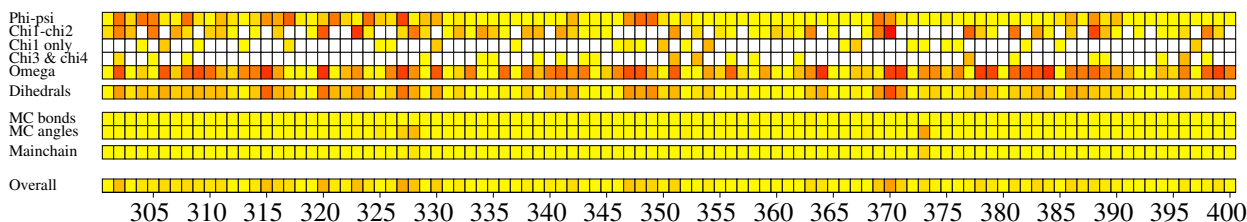
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

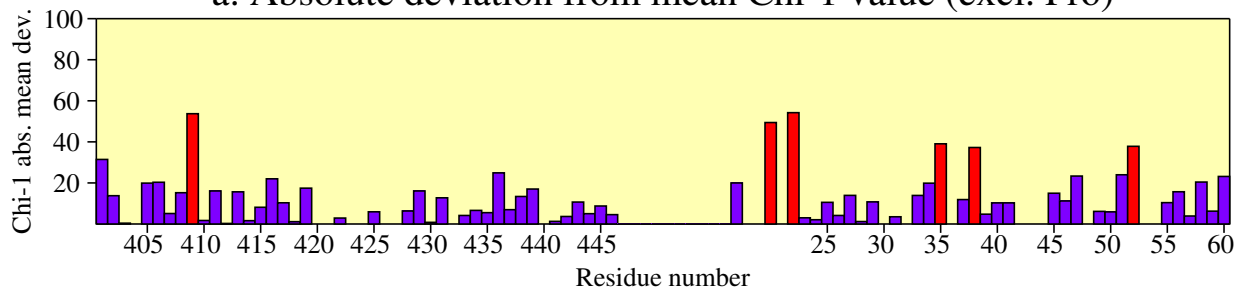


g. G-factors

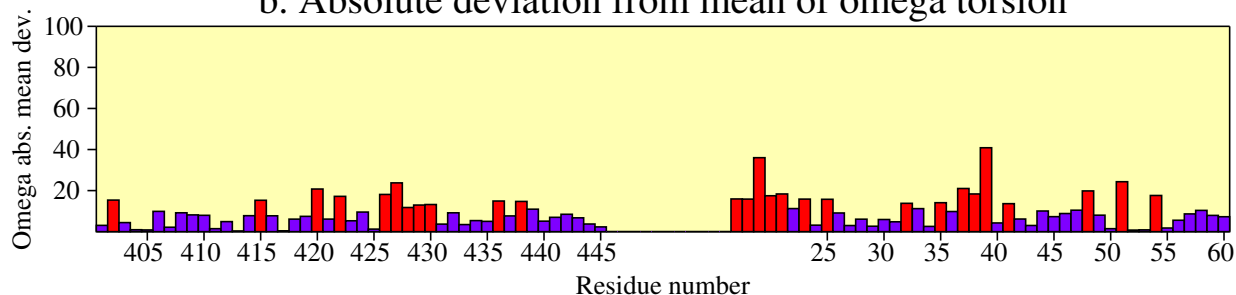


# Residue properties pdb1sqv

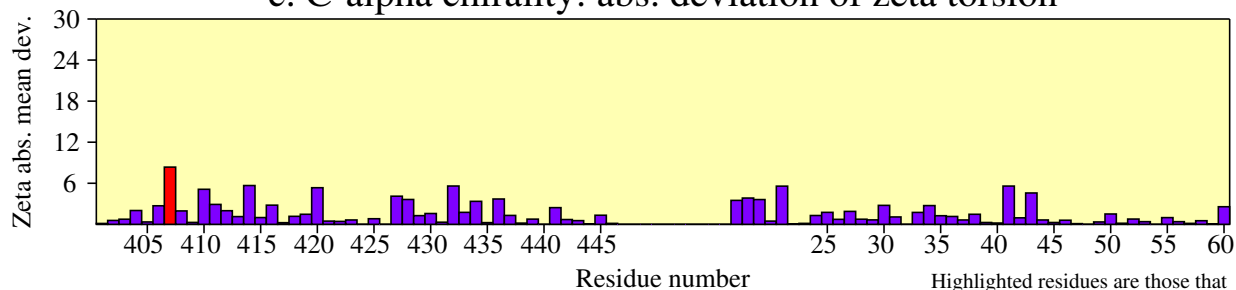
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

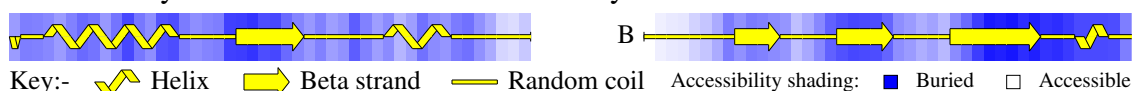


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility



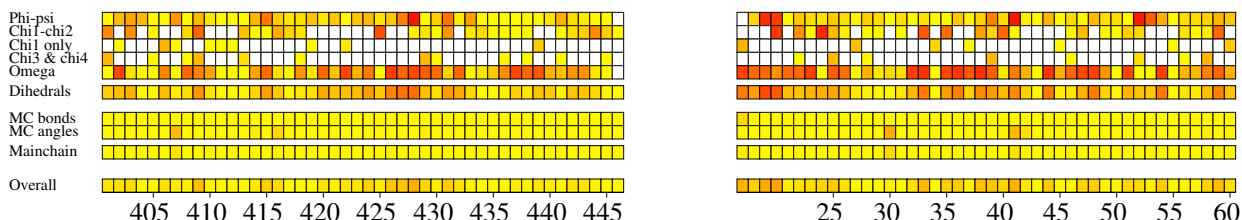
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

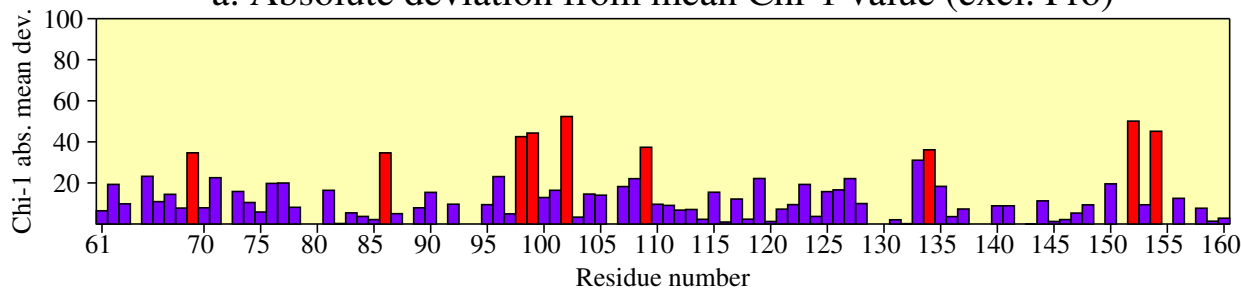


### g. G-factors

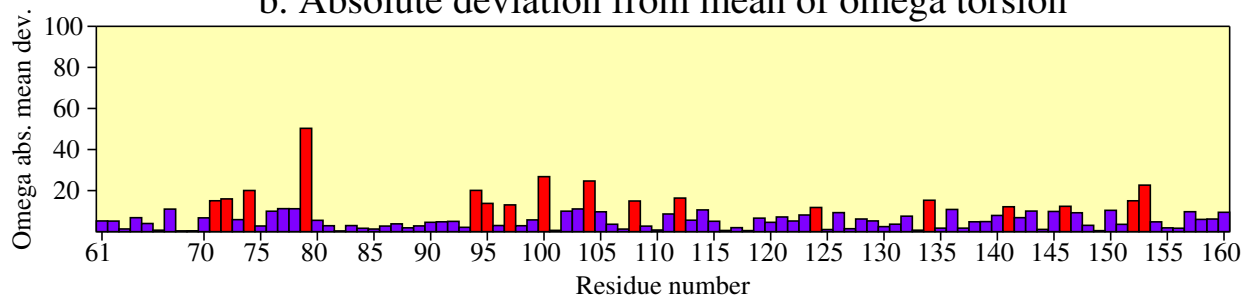


# Residue properties pdb1sqv

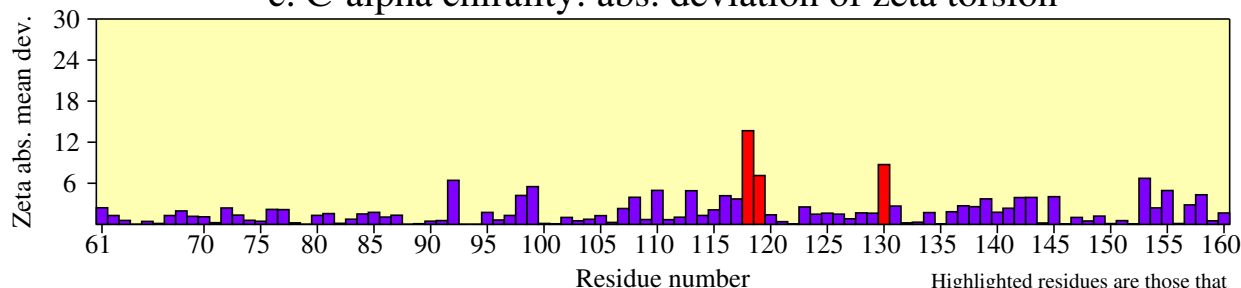
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

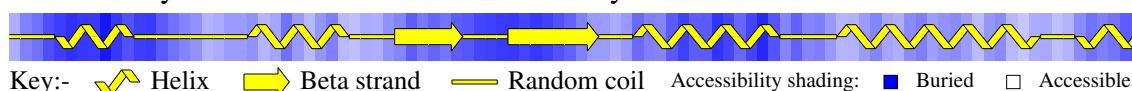


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



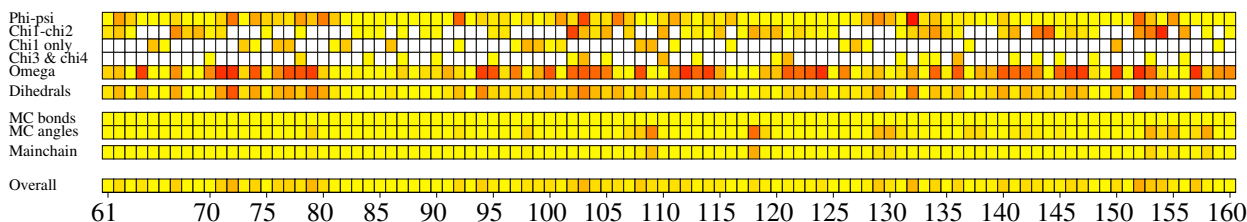
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

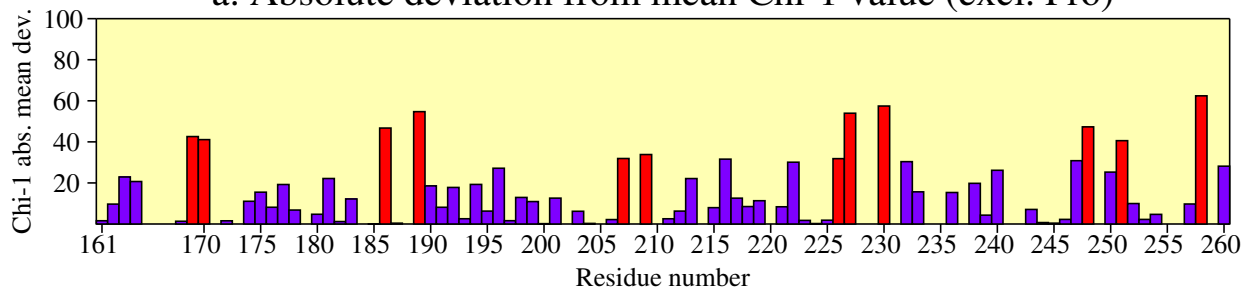


g. G-factors

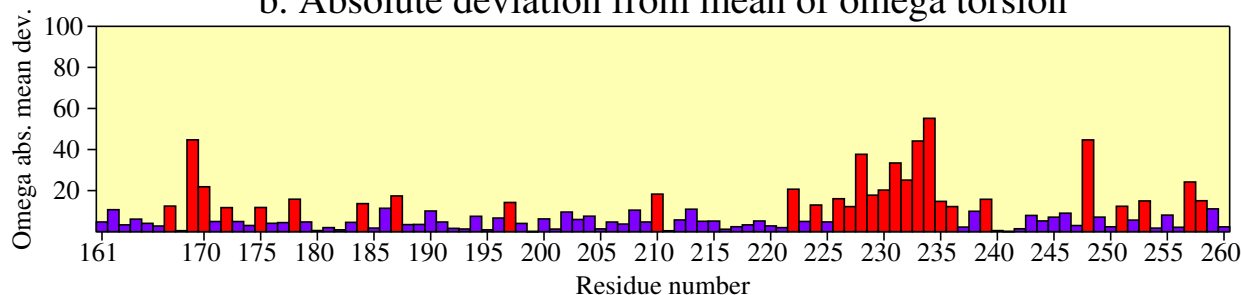


# Residue properties pdb1sqv

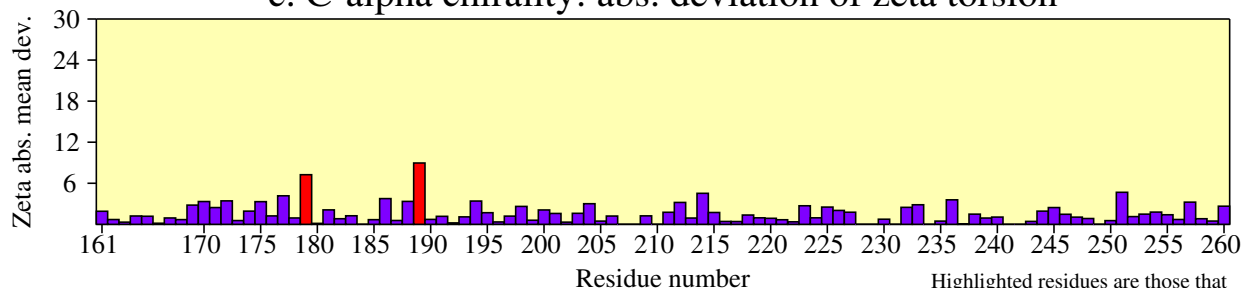
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

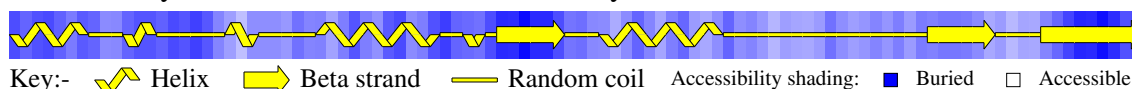


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

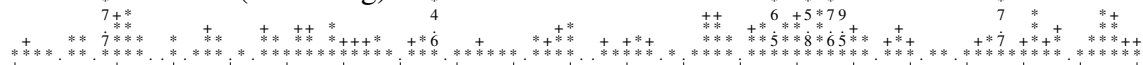
### d. Secondary structure & estimated accessibility



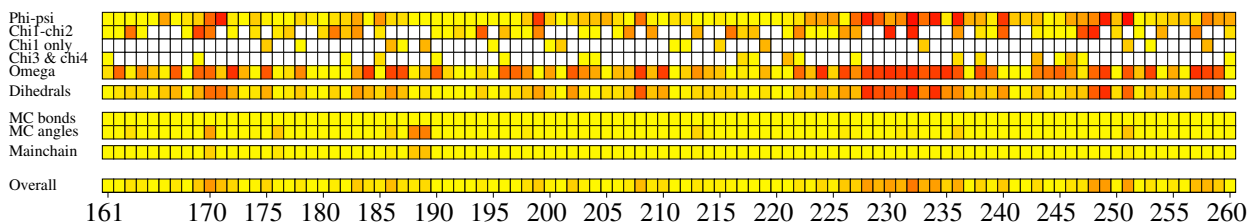
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

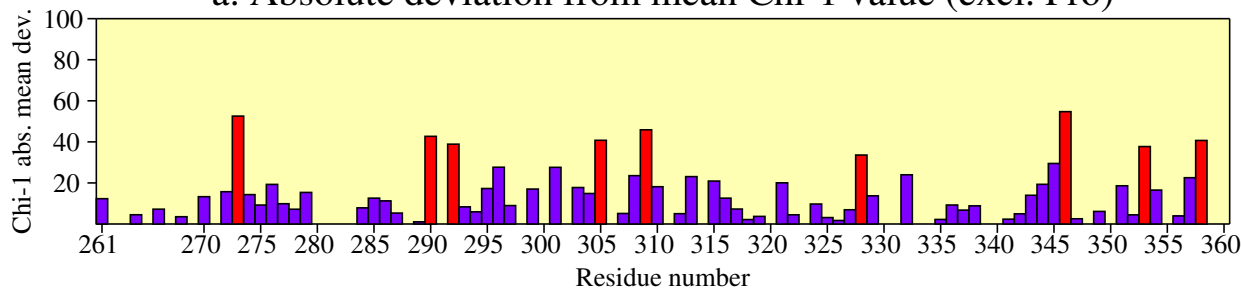


### g. G-factors

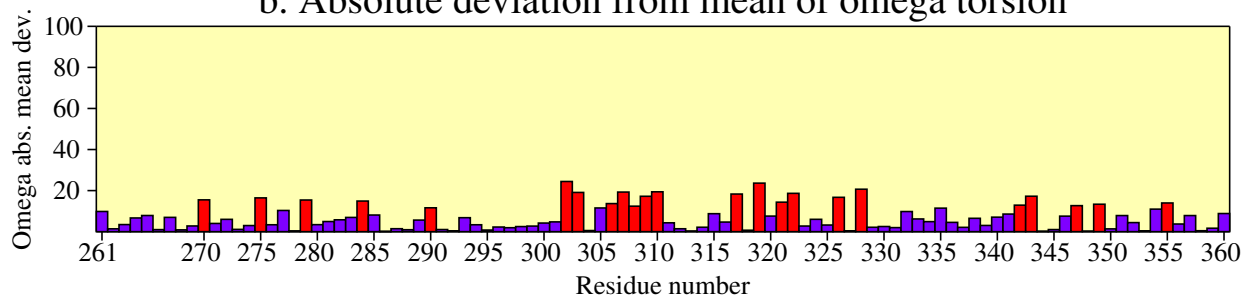


# Residue properties pdb1sqv

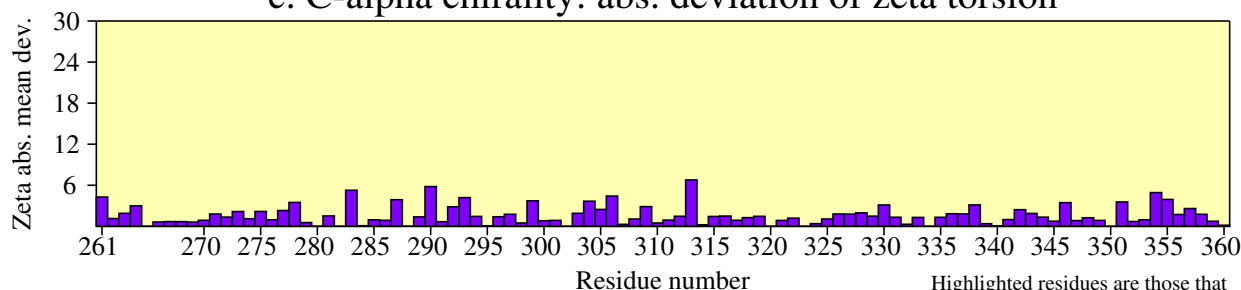
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

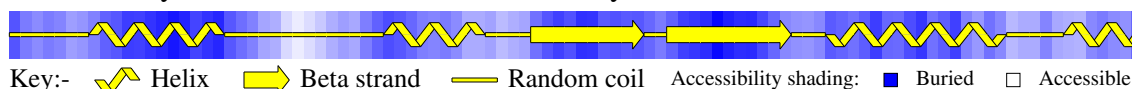


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



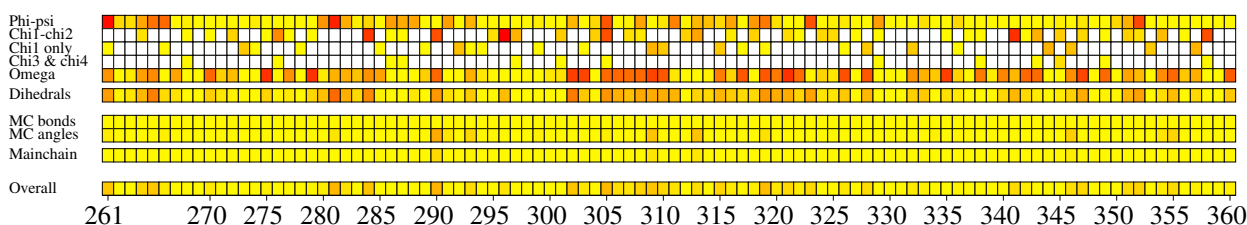
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



g. G-factors

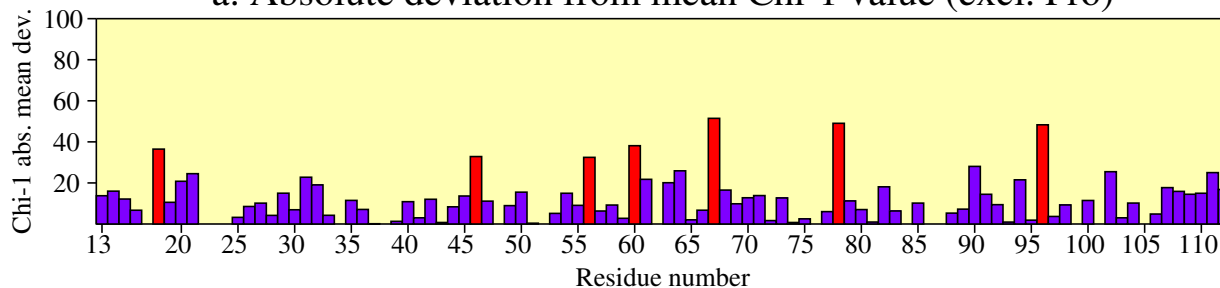




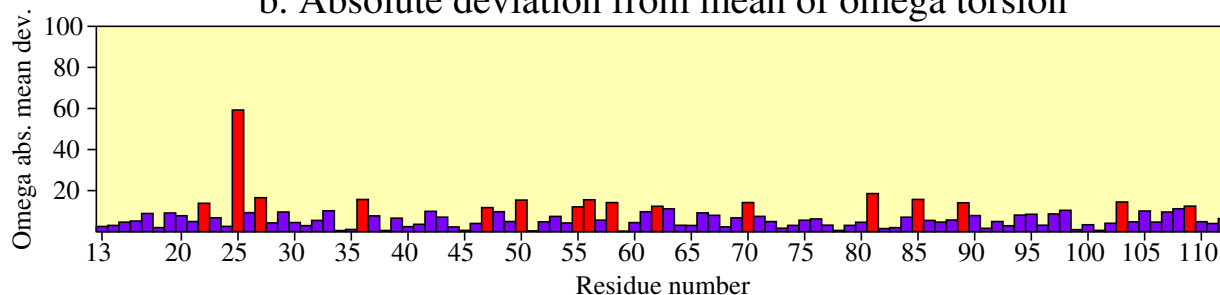


# Residue properties pdb1sqv

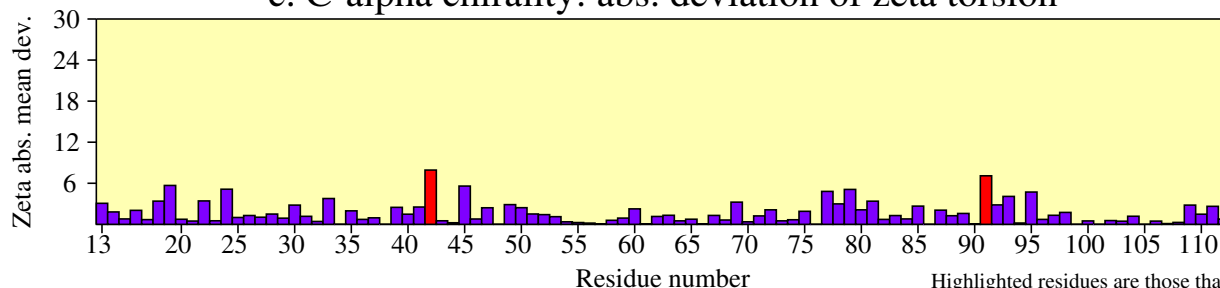
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

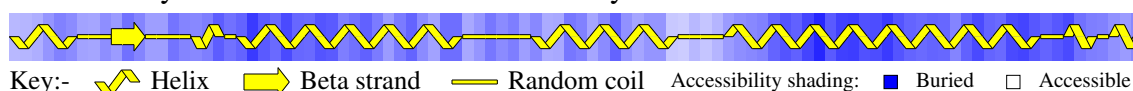


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

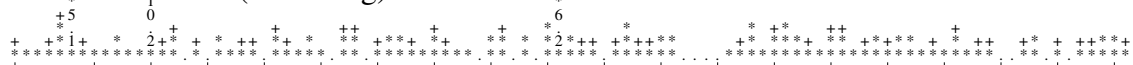
d. Secondary structure & estimated accessibility



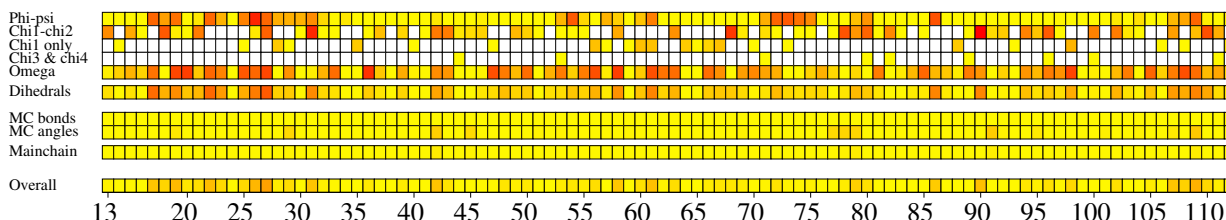
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

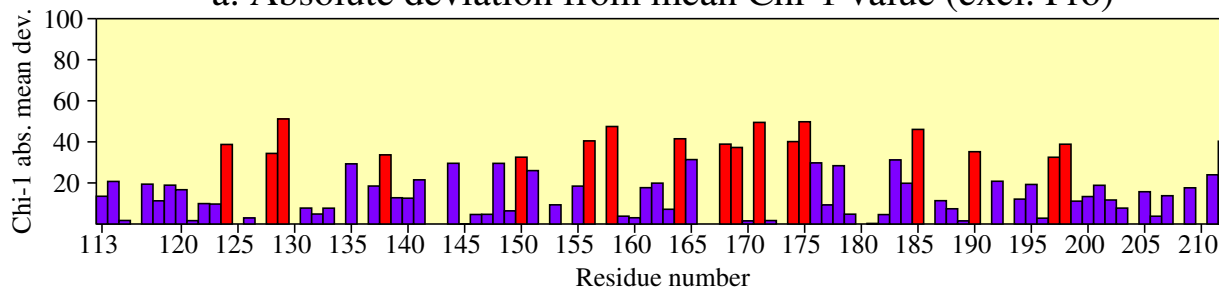


g. G-factors

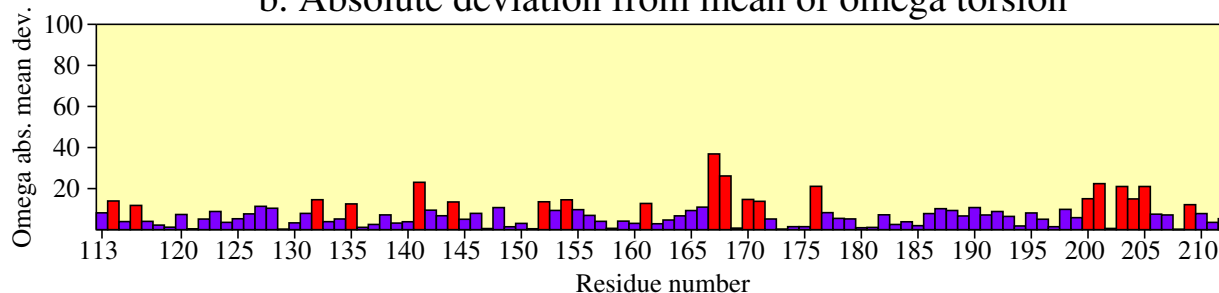


# Residue properties pdb1sqv

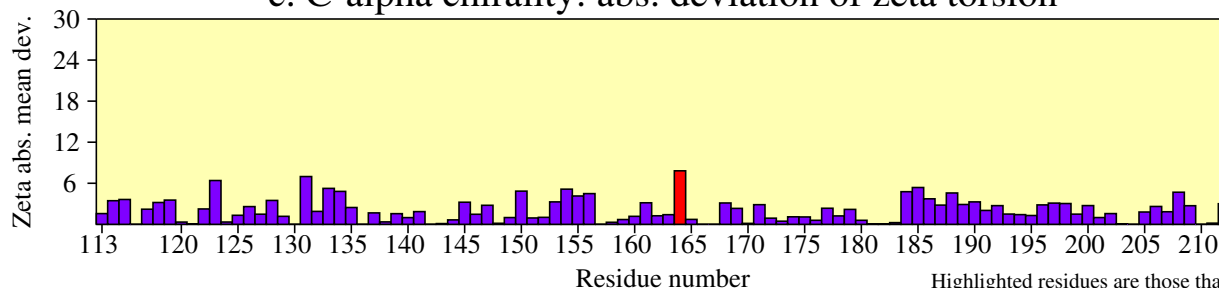
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



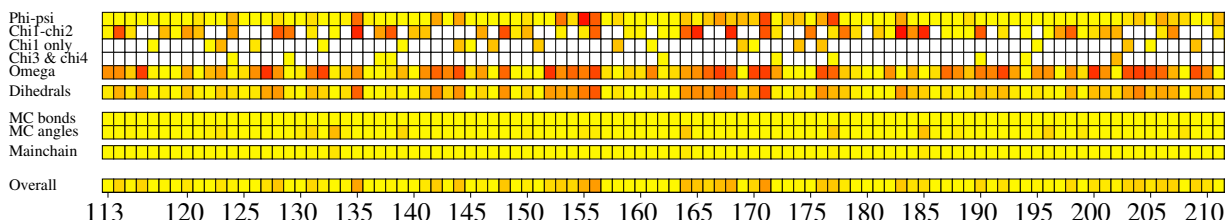
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

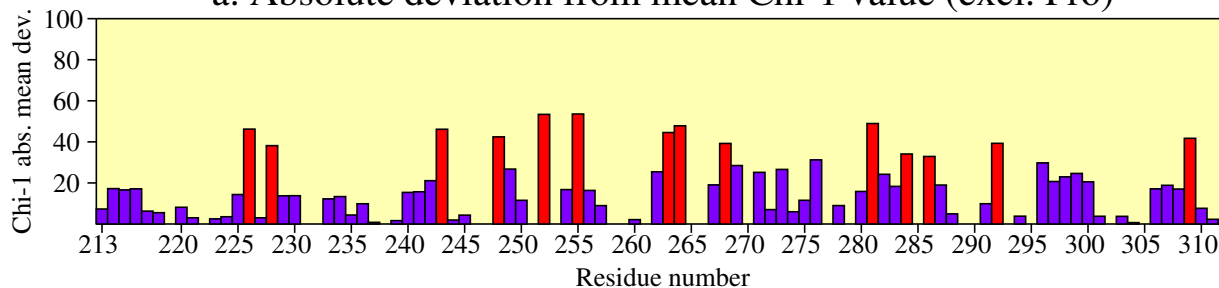


g. G-factors

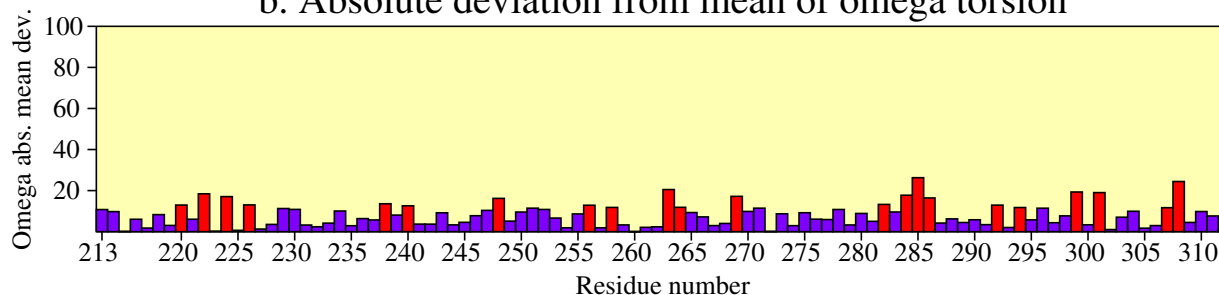


# Residue properties pdb1sqv

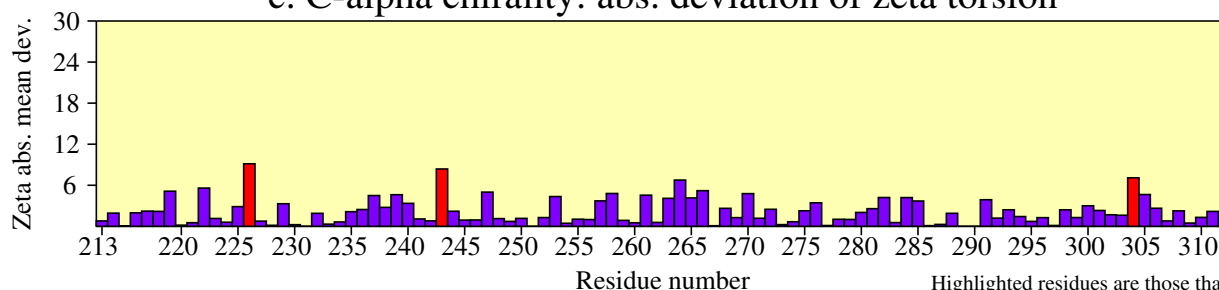
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

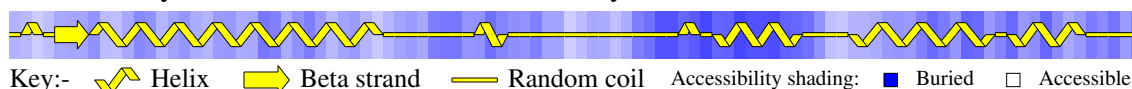


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

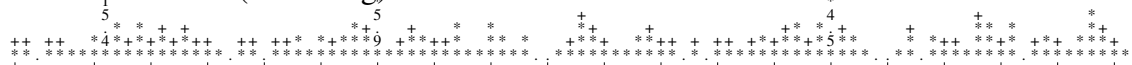


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

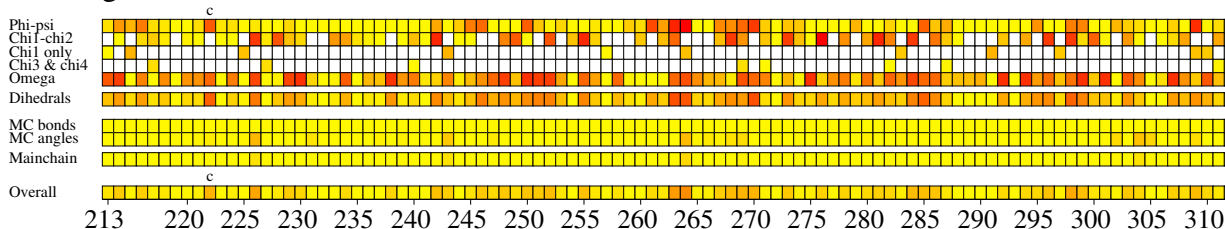
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



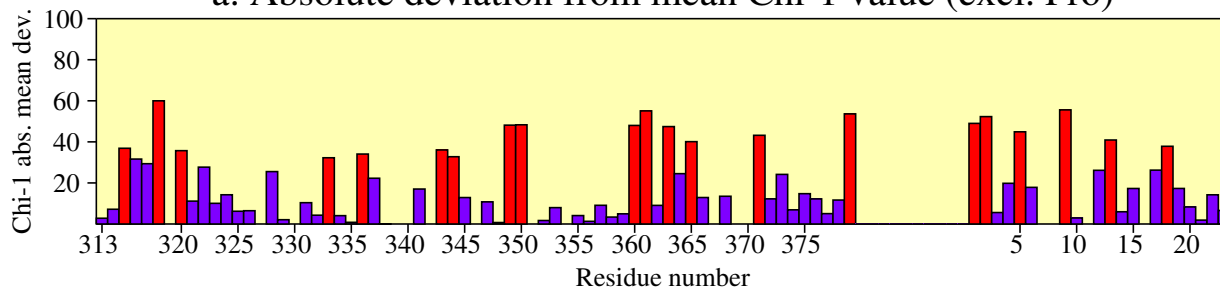
g. G-factors



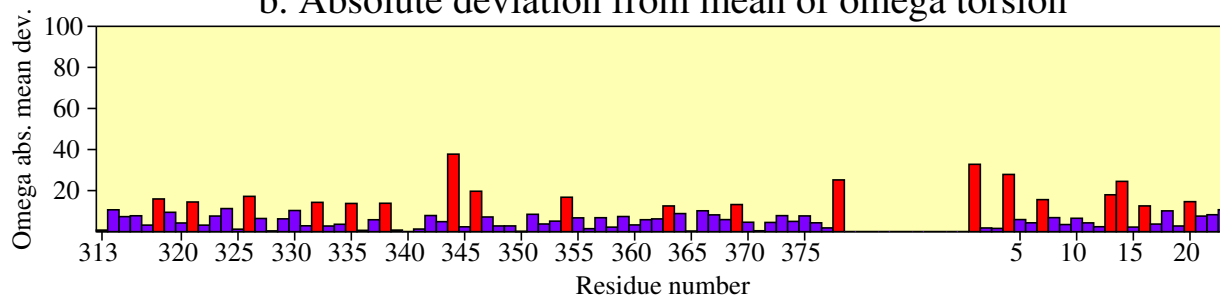
c = cis-peptide

# Residue properties pdb1sqv

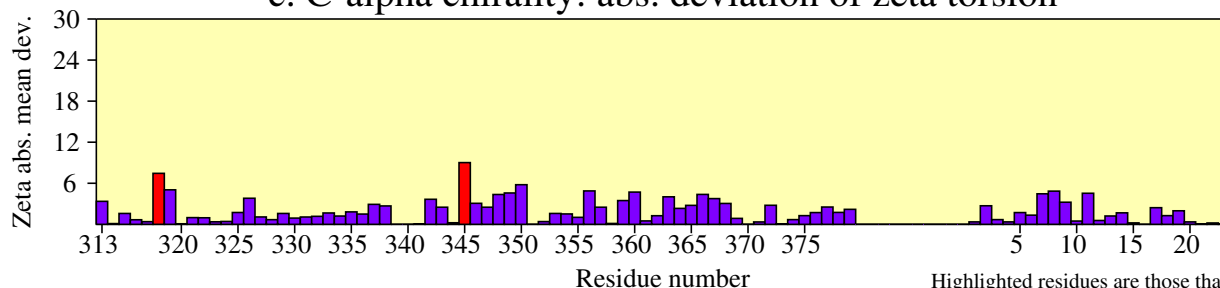
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

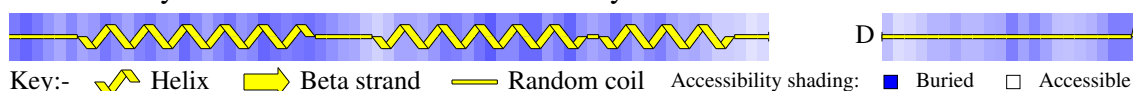


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility



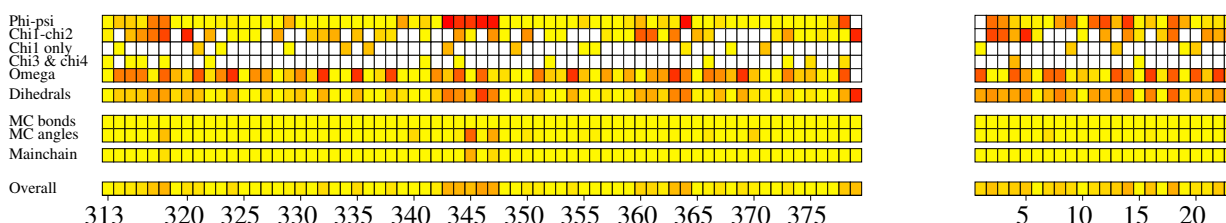
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

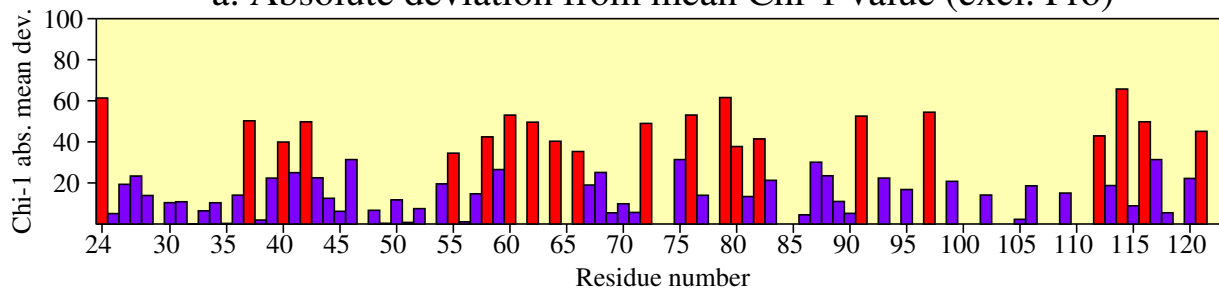


### g. G-factors

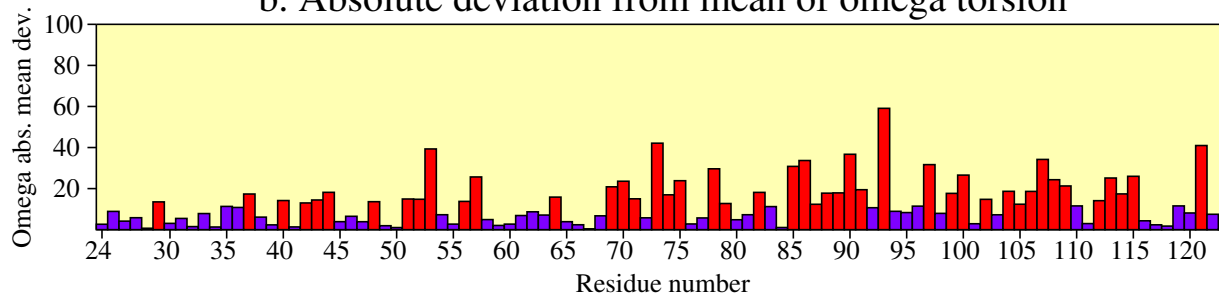


# Residue properties pdb1sqv

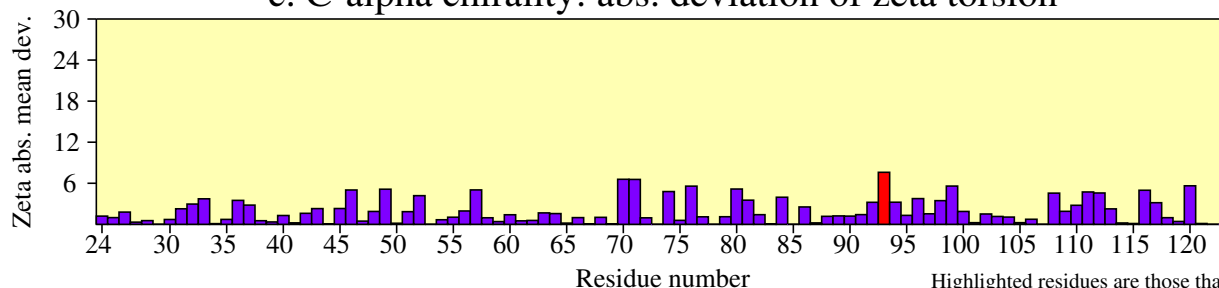
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

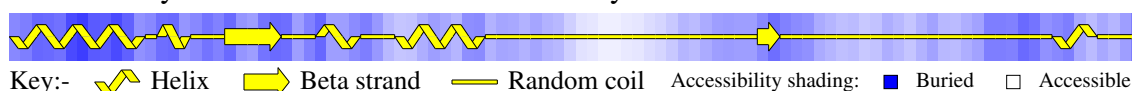


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

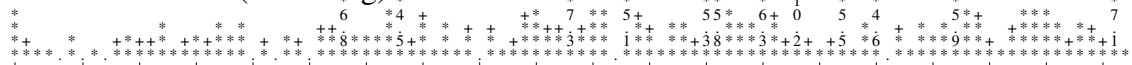
### d. Secondary structure & estimated accessibility



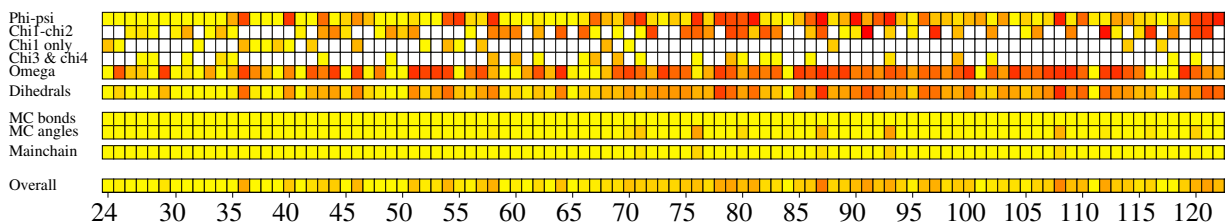
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

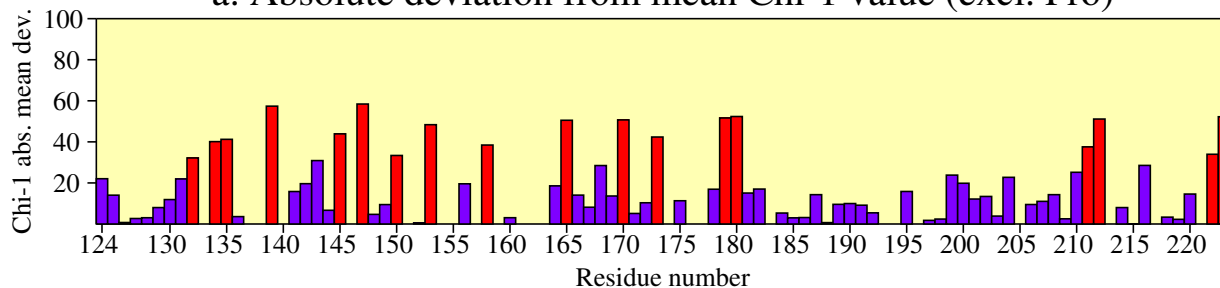


### g. G-factors

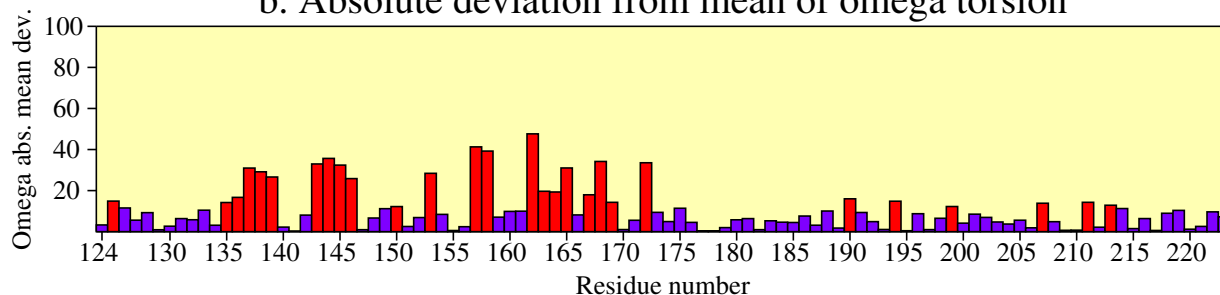


# Residue properties pdb1sqv

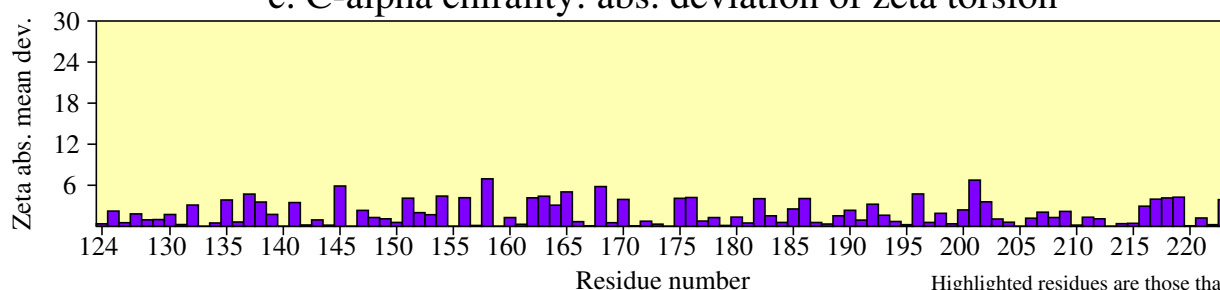
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

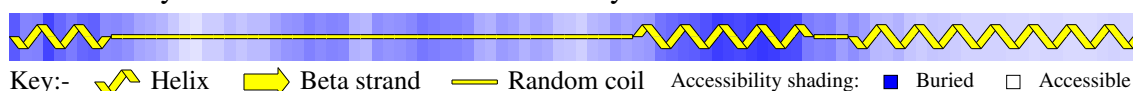


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

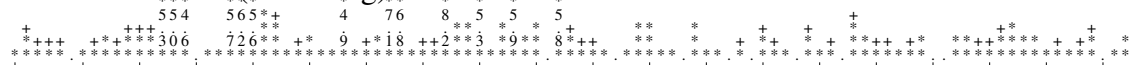
d. Secondary structure & estimated accessibility



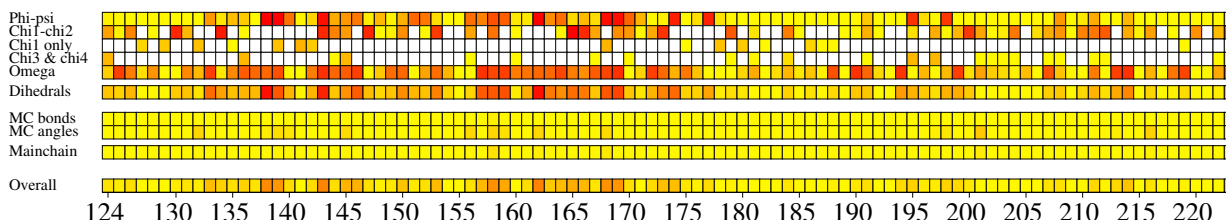
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

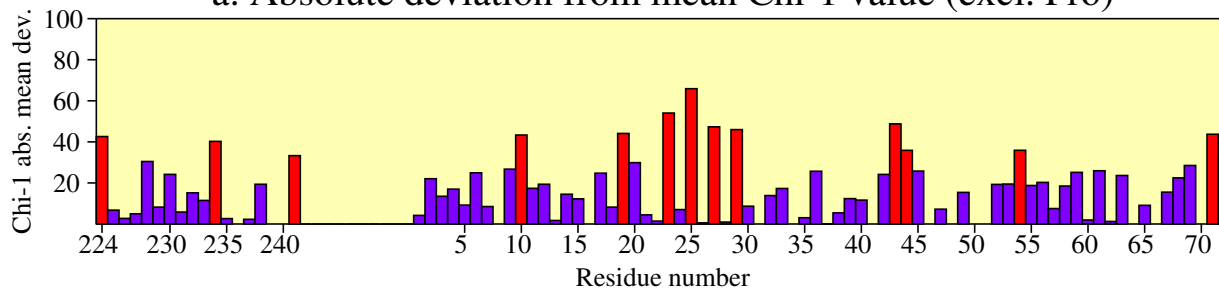


g. G-factors

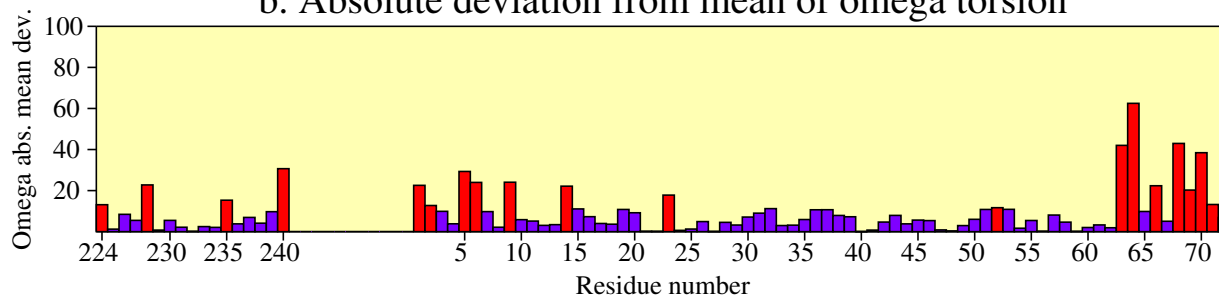


# Residue properties pdb1sqv

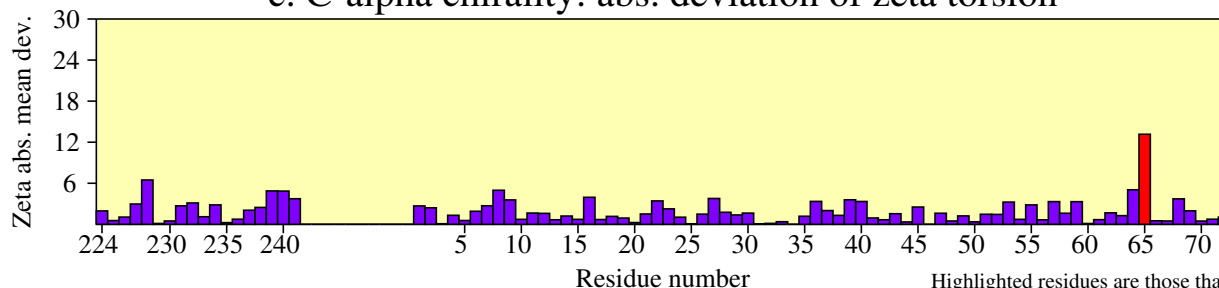
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

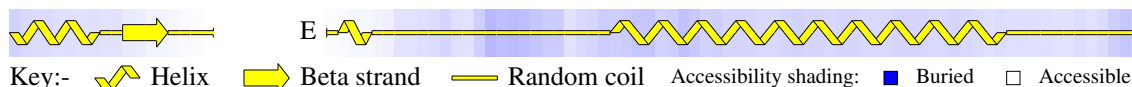


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

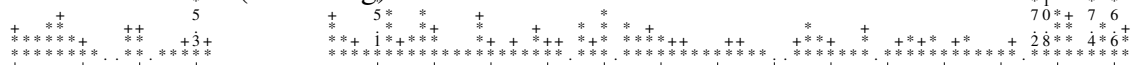
### d. Secondary structure & estimated accessibility



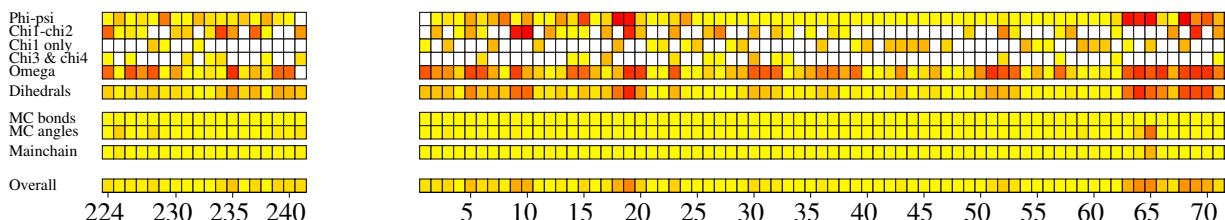
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)



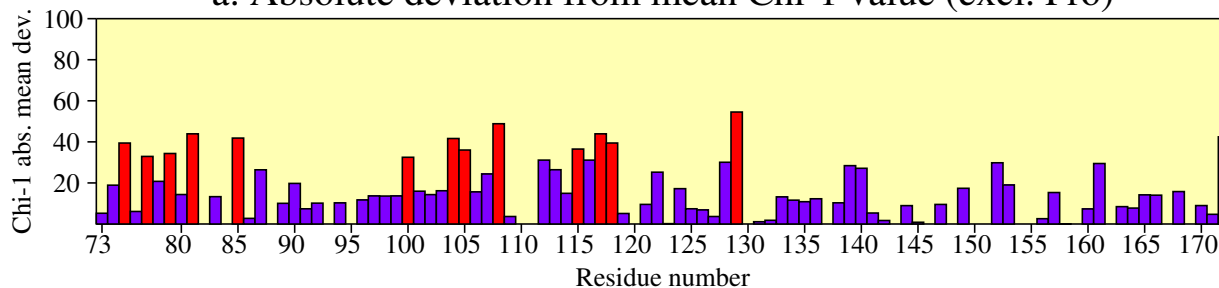
### g. G-factors



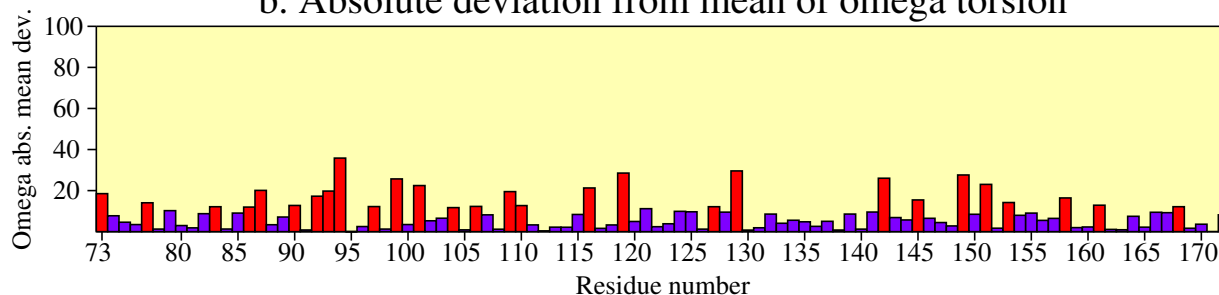


# Residue properties pdb1sqv

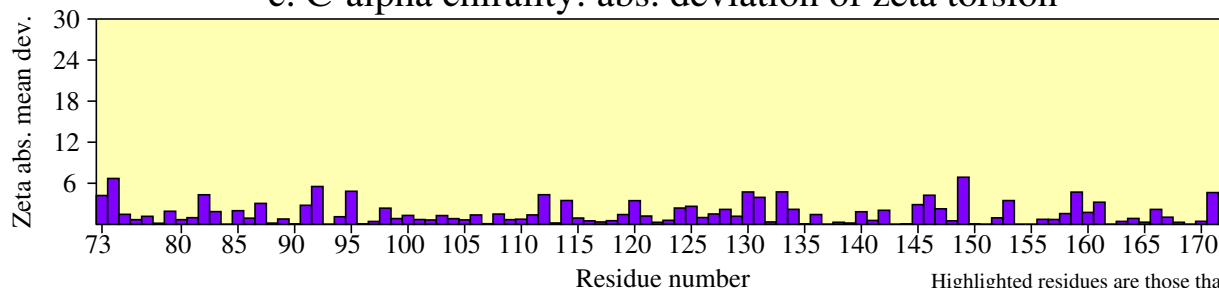
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

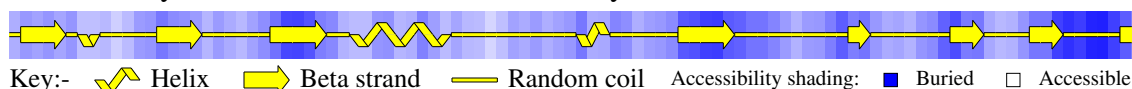


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

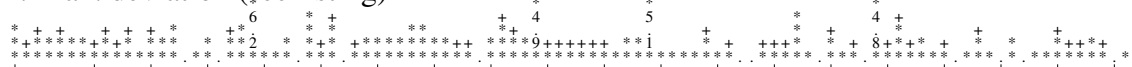
### d. Secondary structure & estimated accessibility



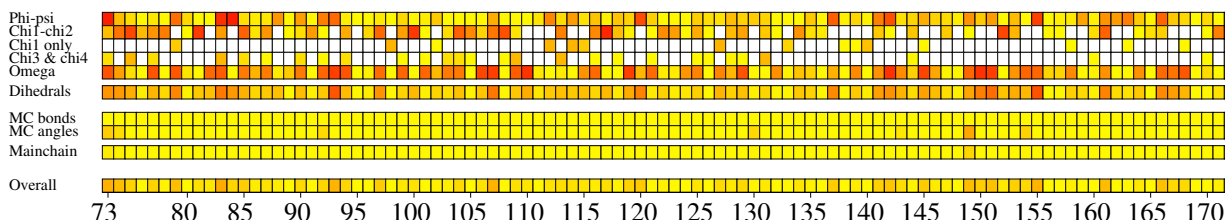
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

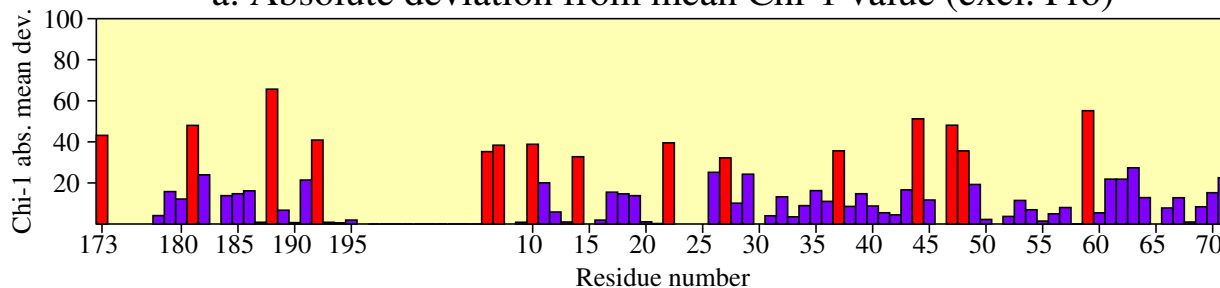


### g. G-factors

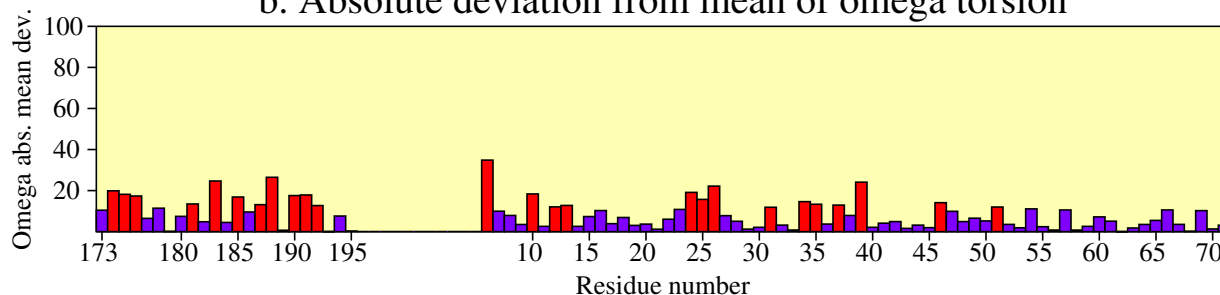


# Residue properties pdb1sqv

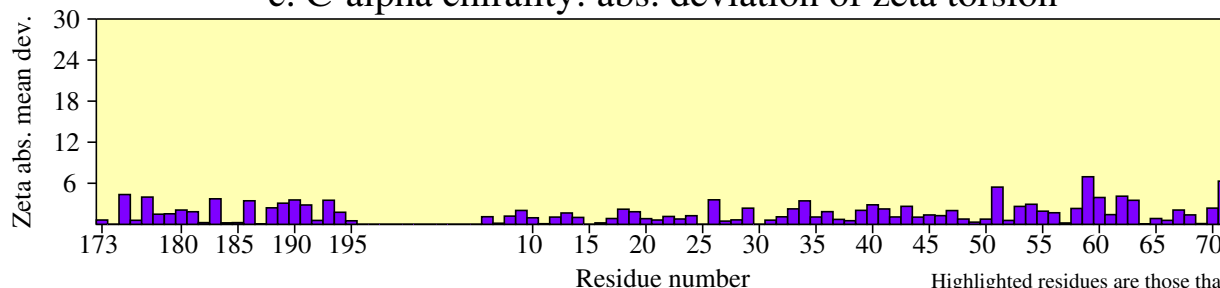
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

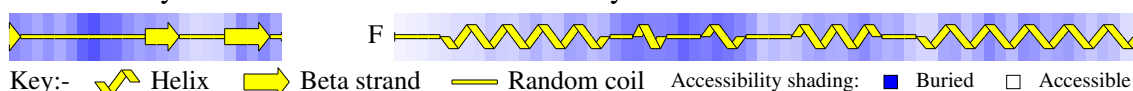


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility



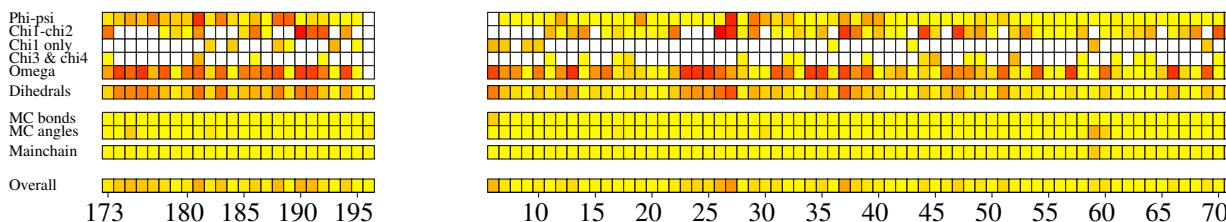
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

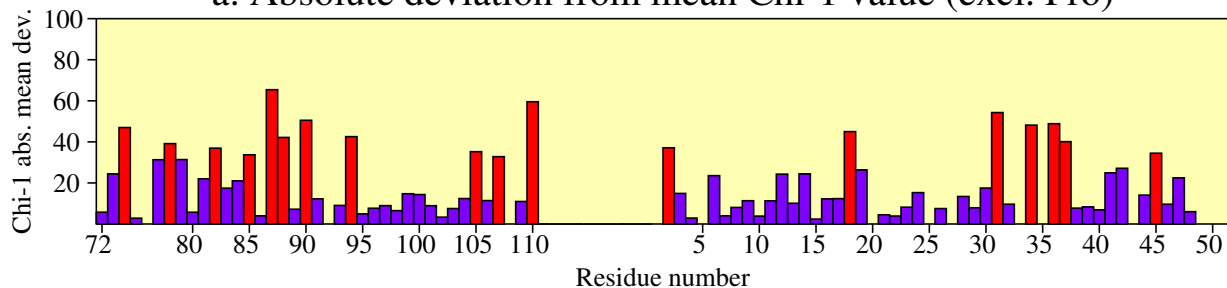


### g. G-factors

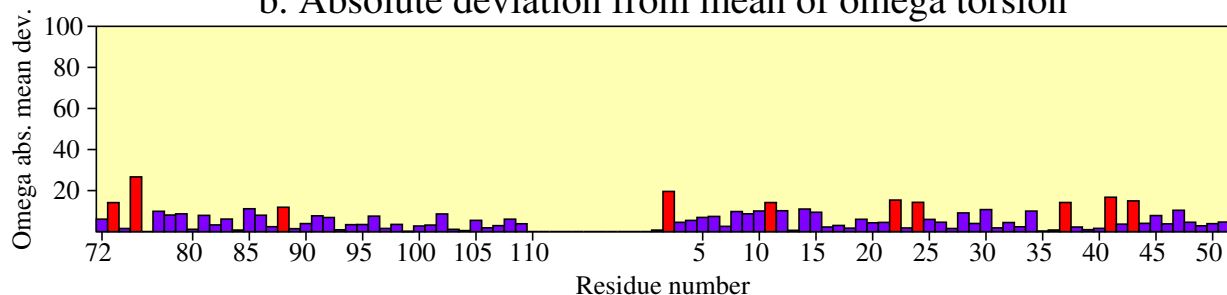


# Residue properties pdb1sqv

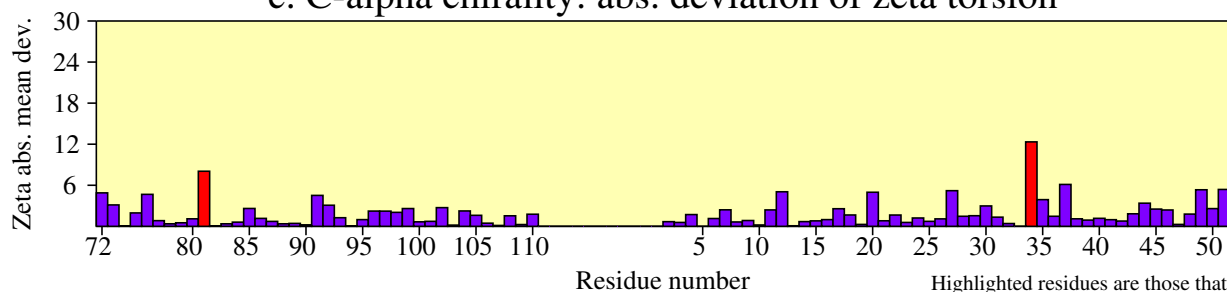
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

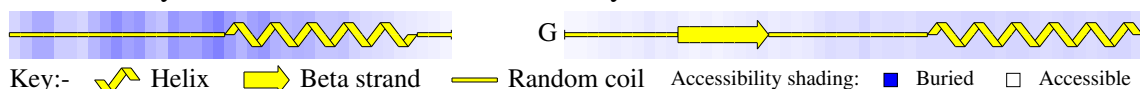


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility



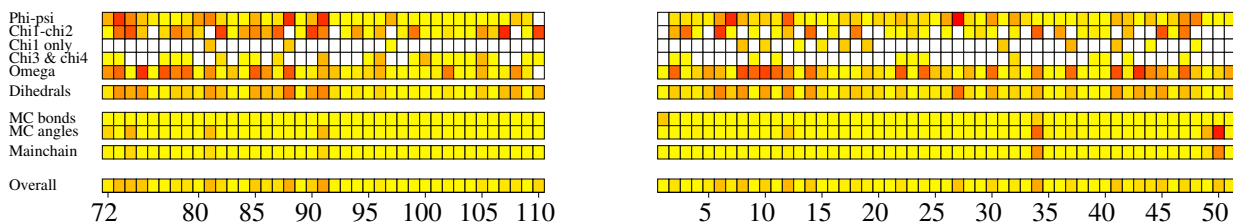
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

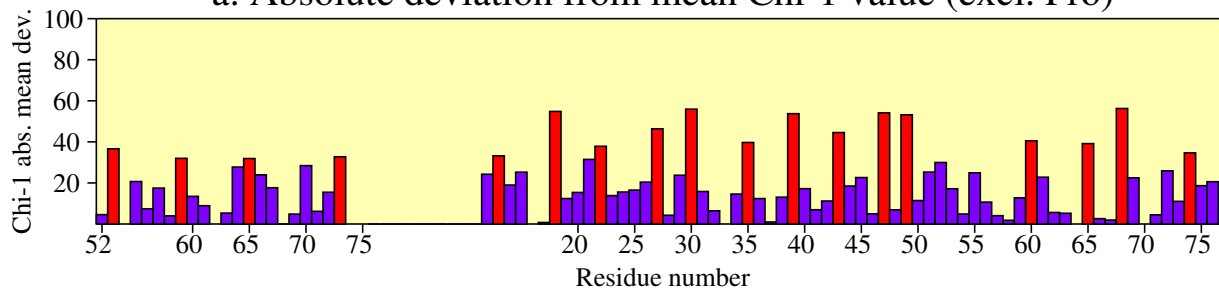


### g. G-factors

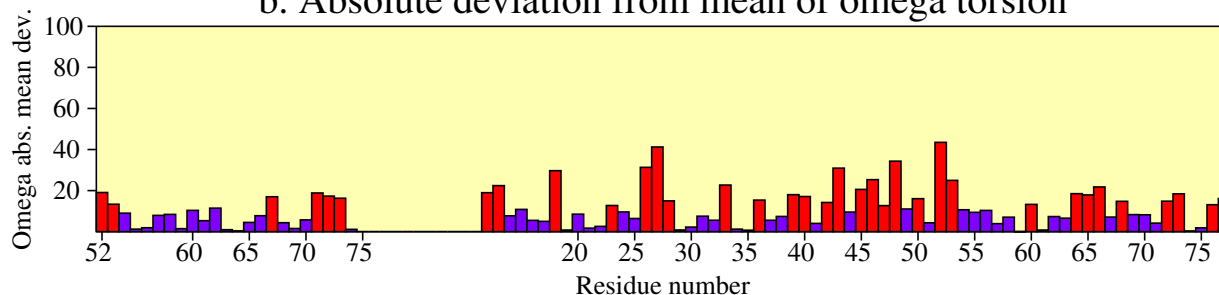


# Residue properties pdb1sqv

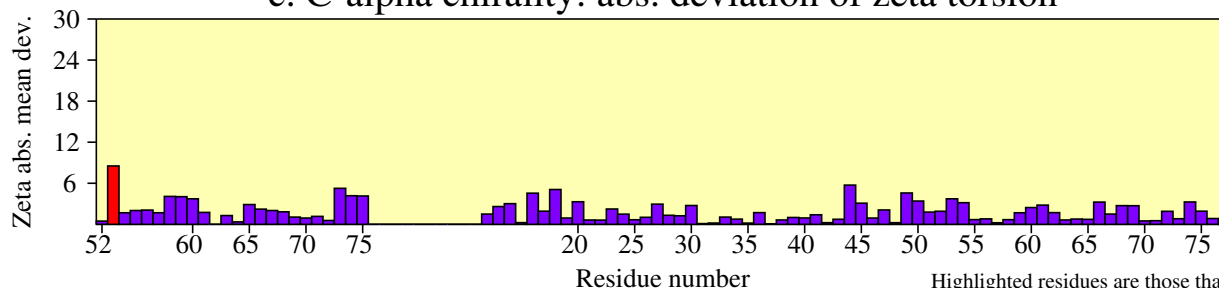
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

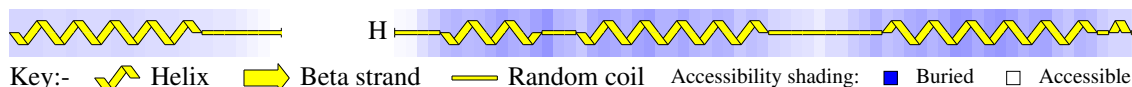


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

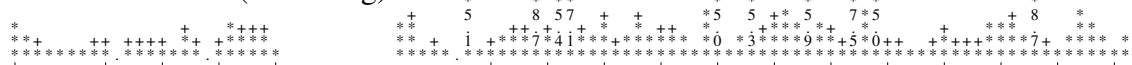
### d. Secondary structure & estimated accessibility



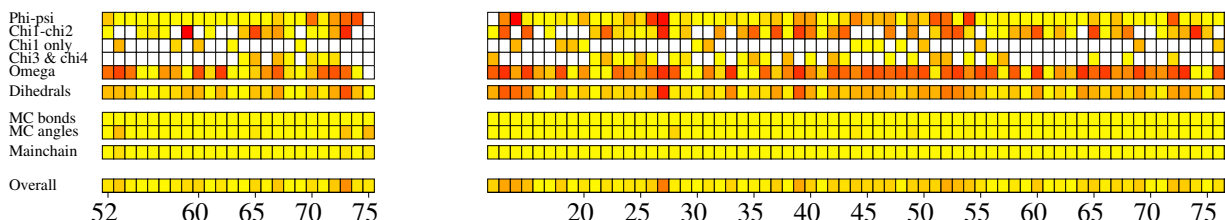
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

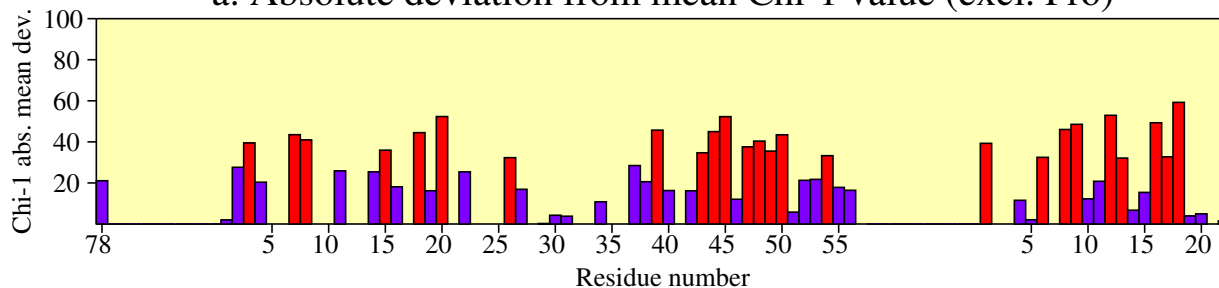


### g. G-factors

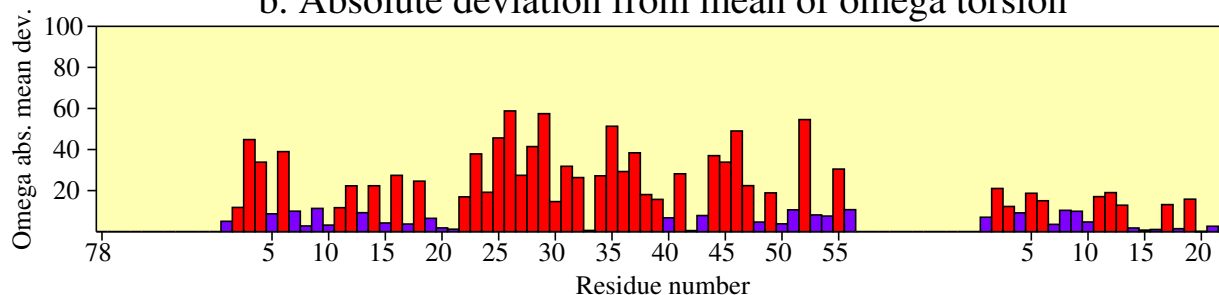


# Residue properties pdb1sqv

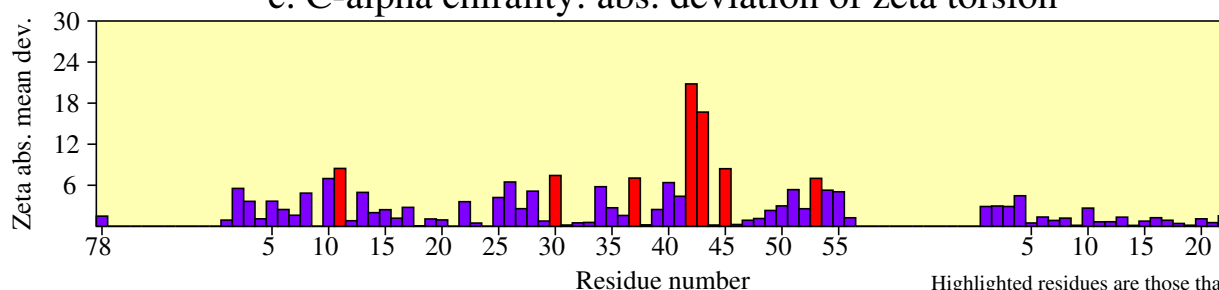
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

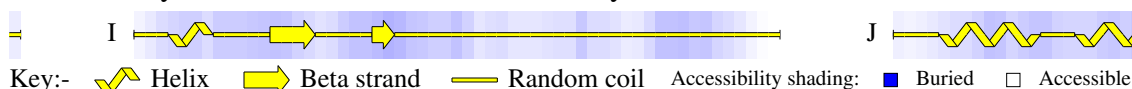


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

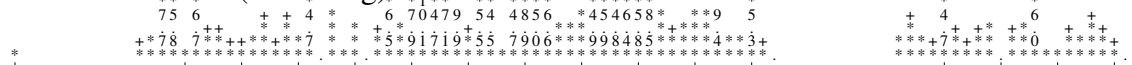
d. Secondary structure & estimated accessibility



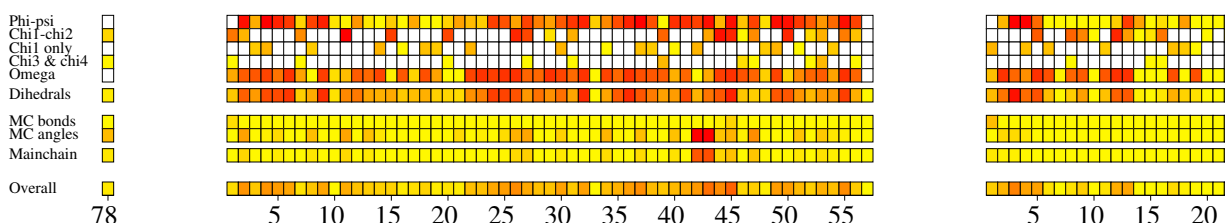
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

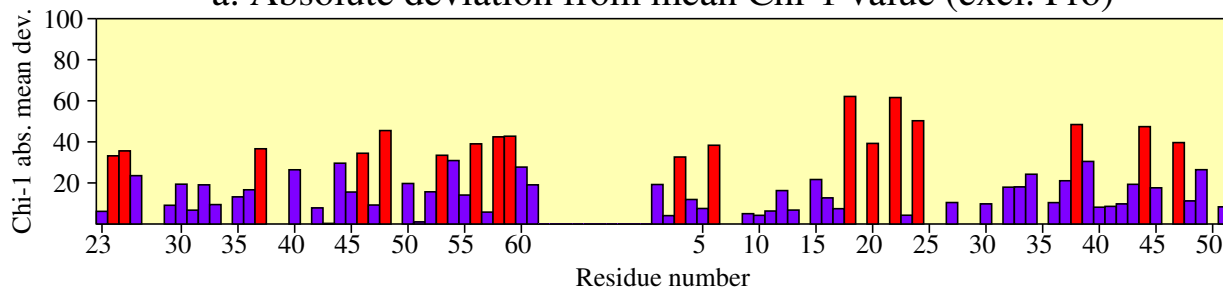


g. G-factors

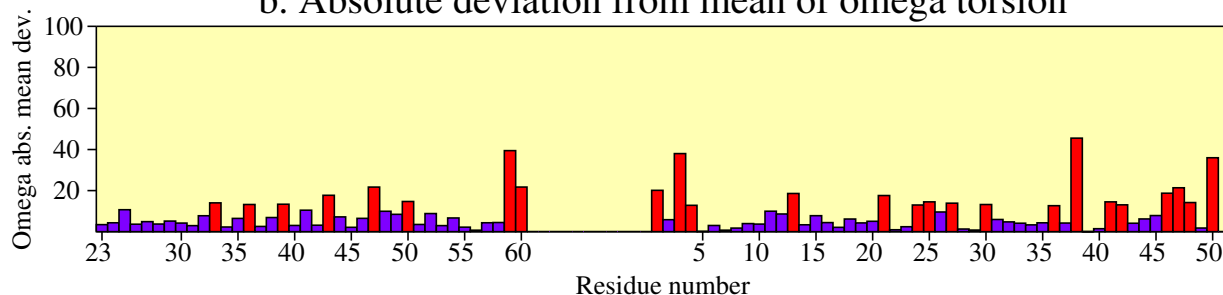


# Residue properties pdb1sqv

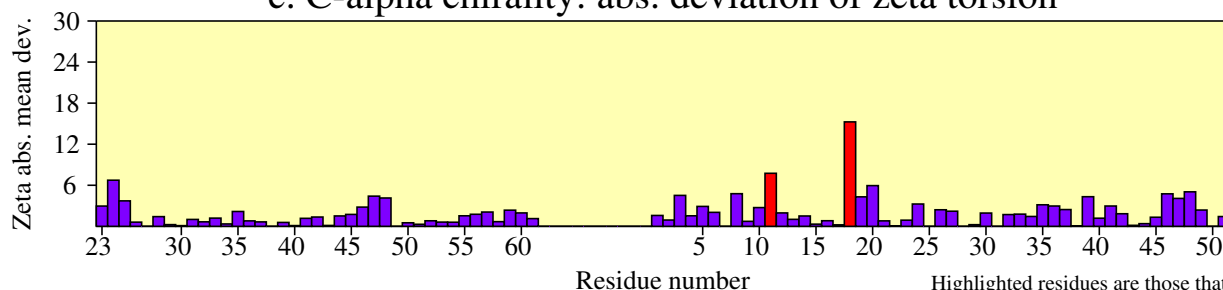
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

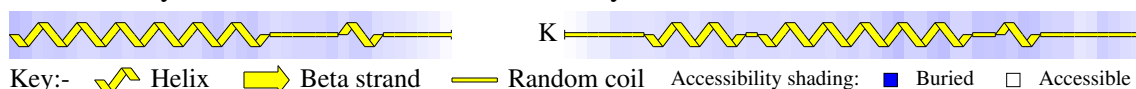


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

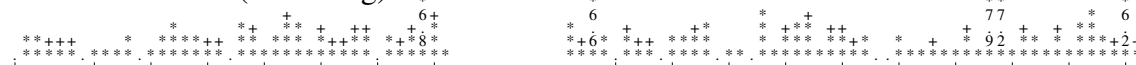
### d. Secondary structure & estimated accessibility



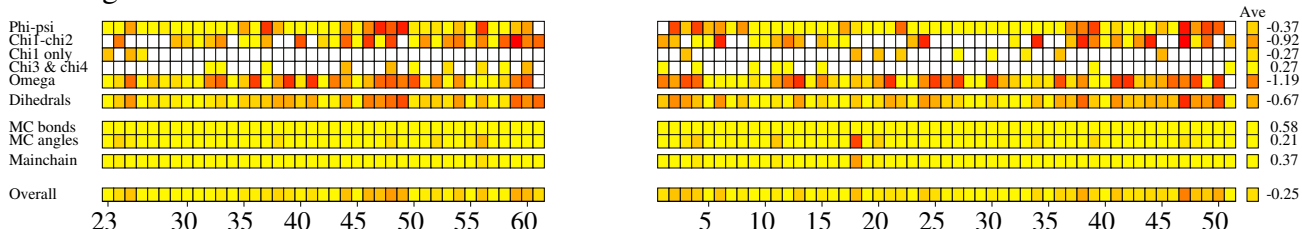
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

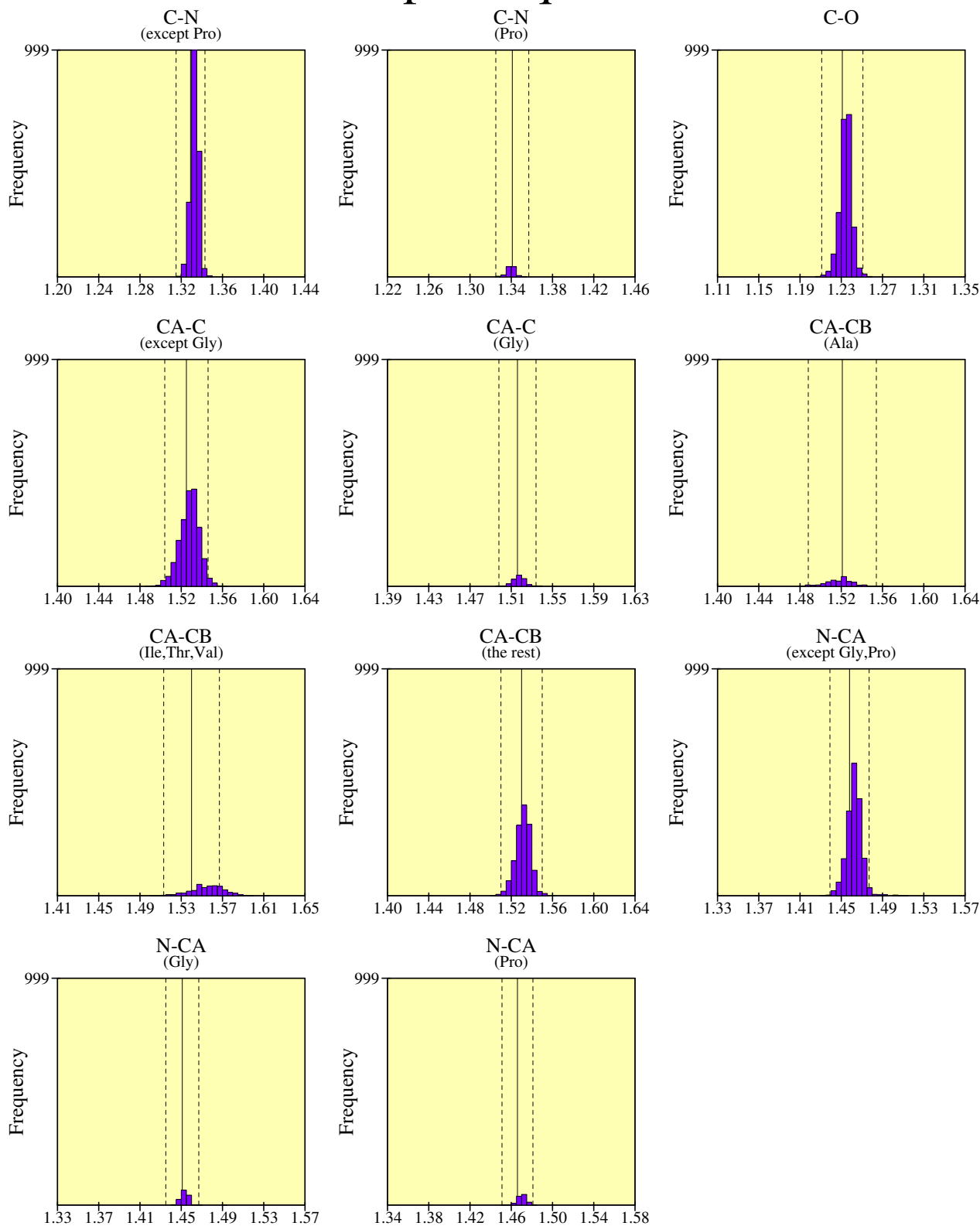


### g. G-factors



# Main-chain bond lengths

## pdb1sqv

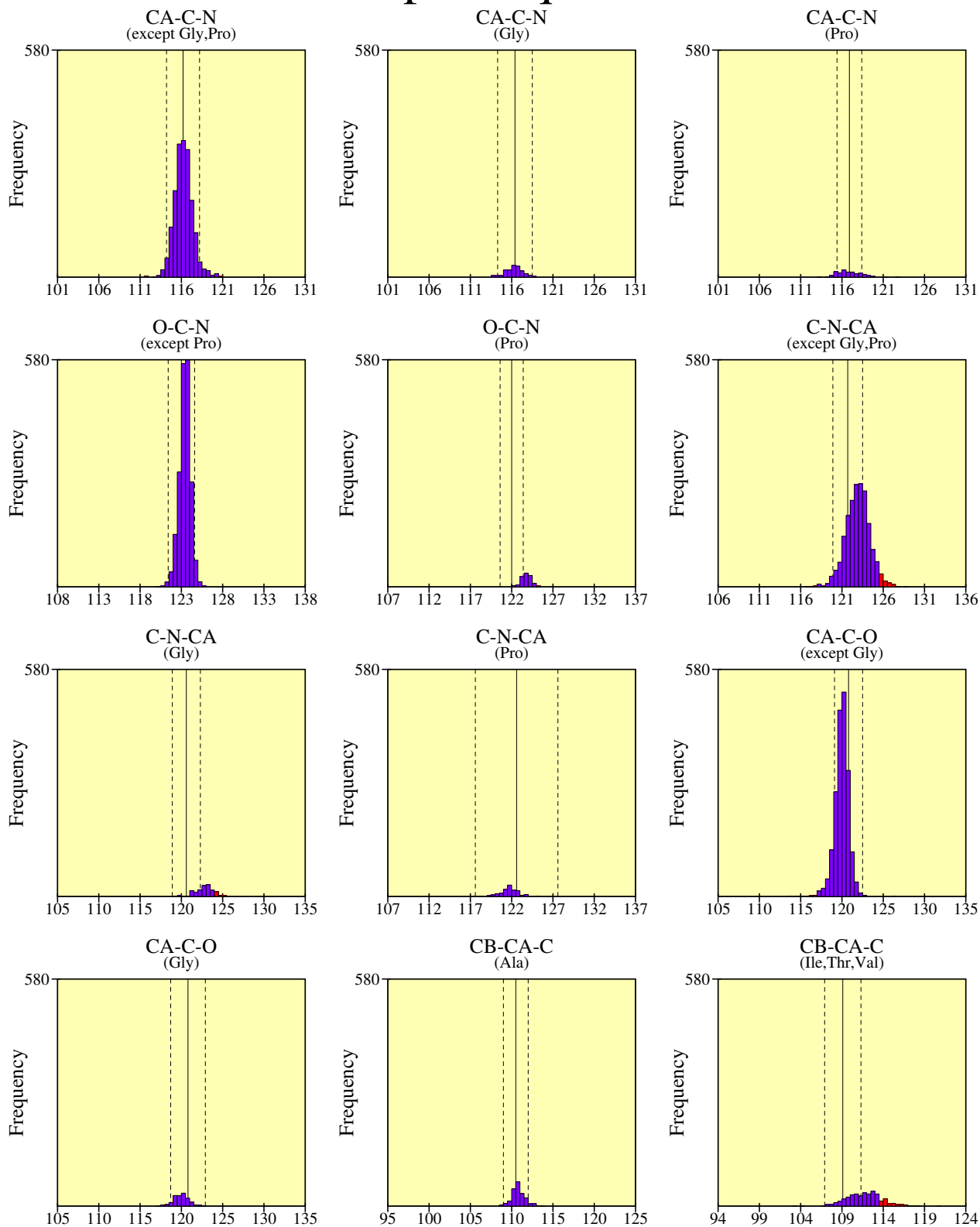


Black bars > 2.0 st. devs. from mean.

Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

# Main-chain bond angles

## pdb1sqv



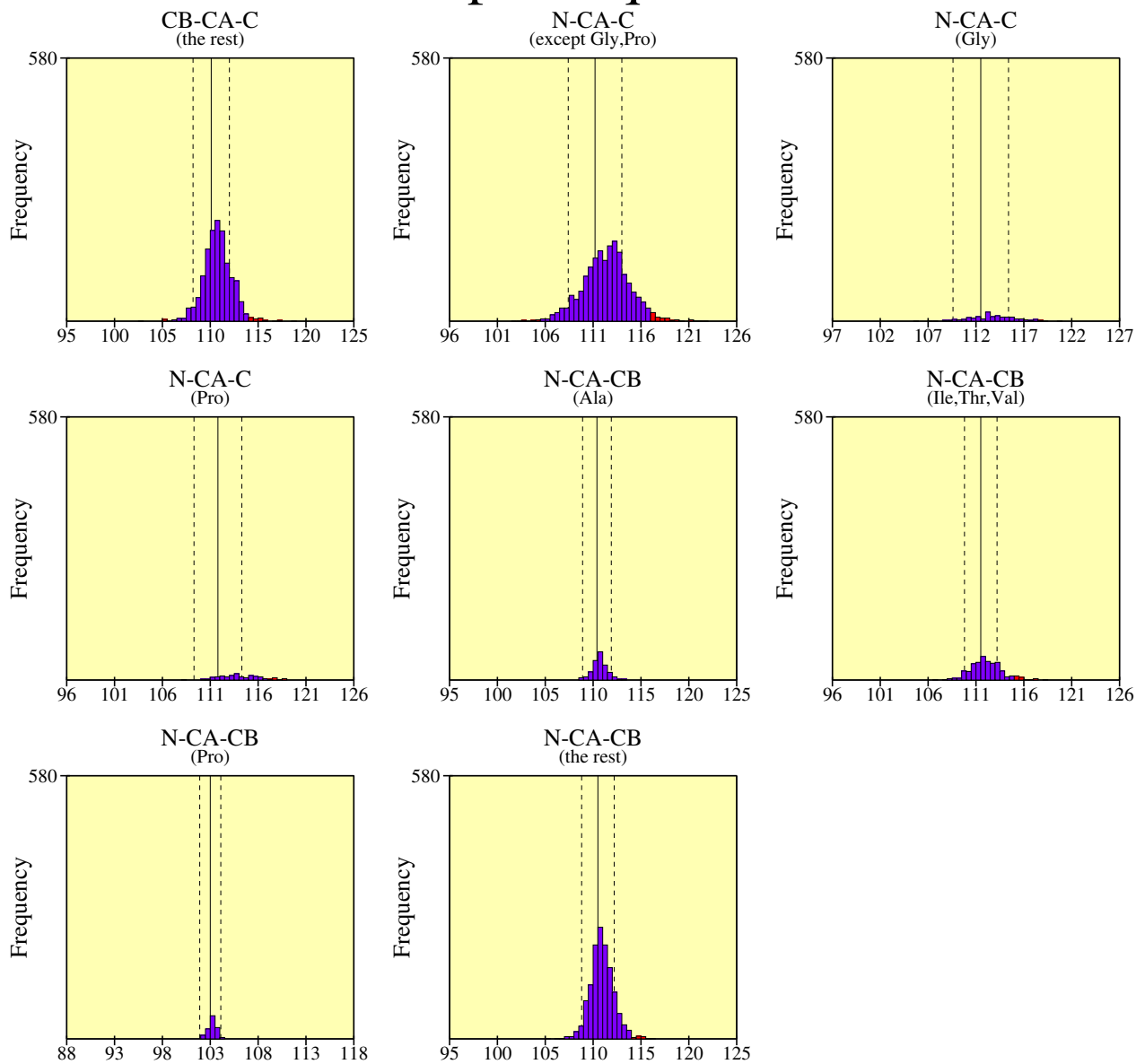
Black bars > 2.0 st. devs. from mean.

Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.



# Main-chain bond angles

## pdb1sqv

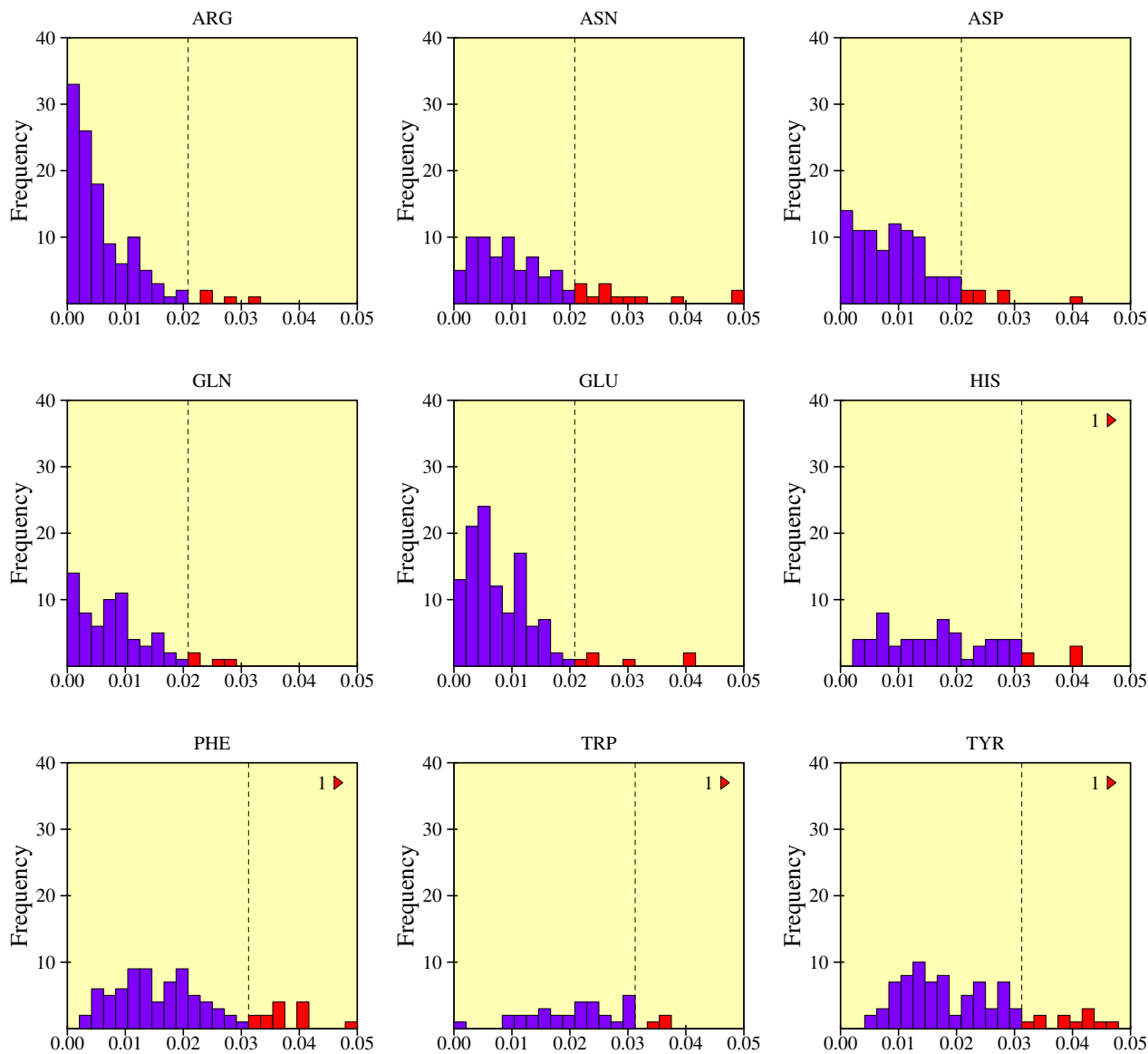


Black bars > 2.0 st. devs. from mean.

Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

# RMS distances from planarity

## pdb1sqv



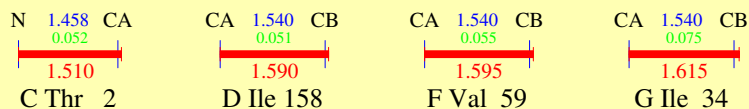
Histograms showing RMS distances of planar atoms from best-fit plane.  
 Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

▶ signifies data points off the graph in the direction shown.

# Distorted geometry

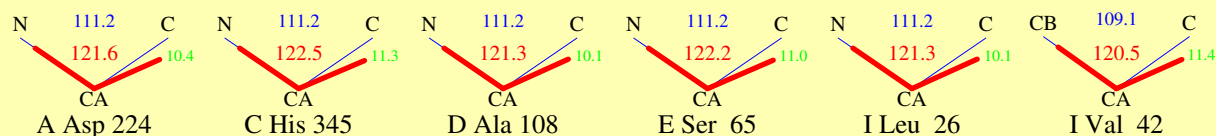
## pdb1sqv

### Main-chain bond lengths



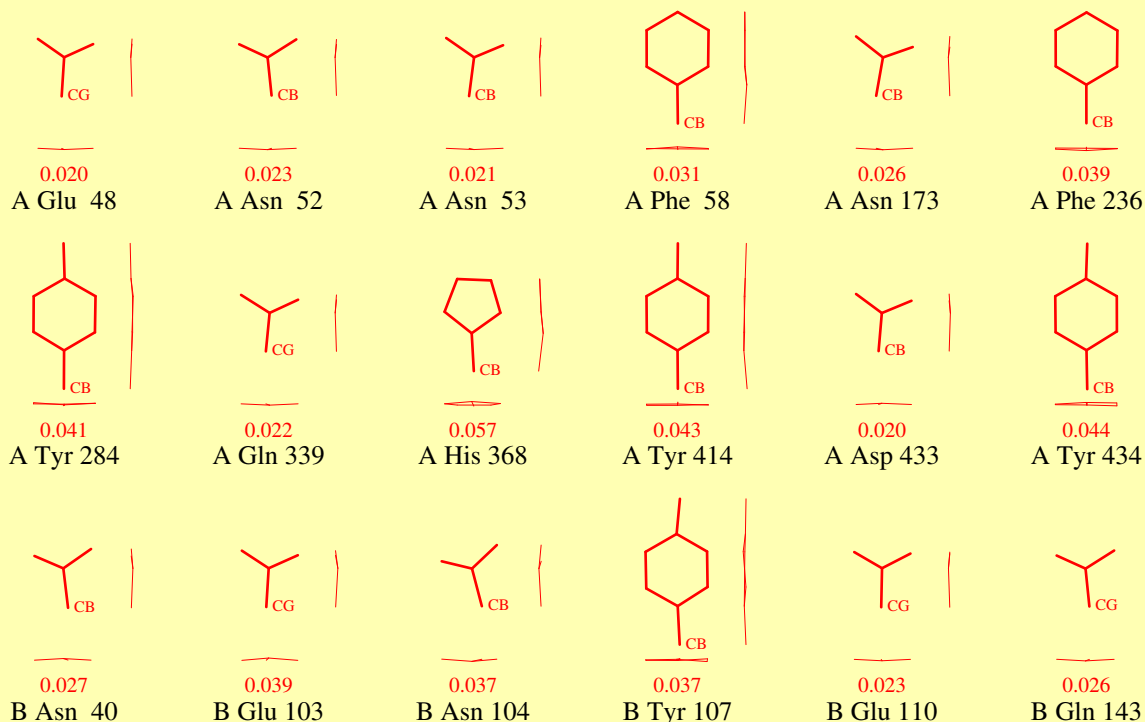
Bonds differing by > 0.05A from small-molecule values. Values shown: "ideal", difference, actual

### Main-chain bond angles



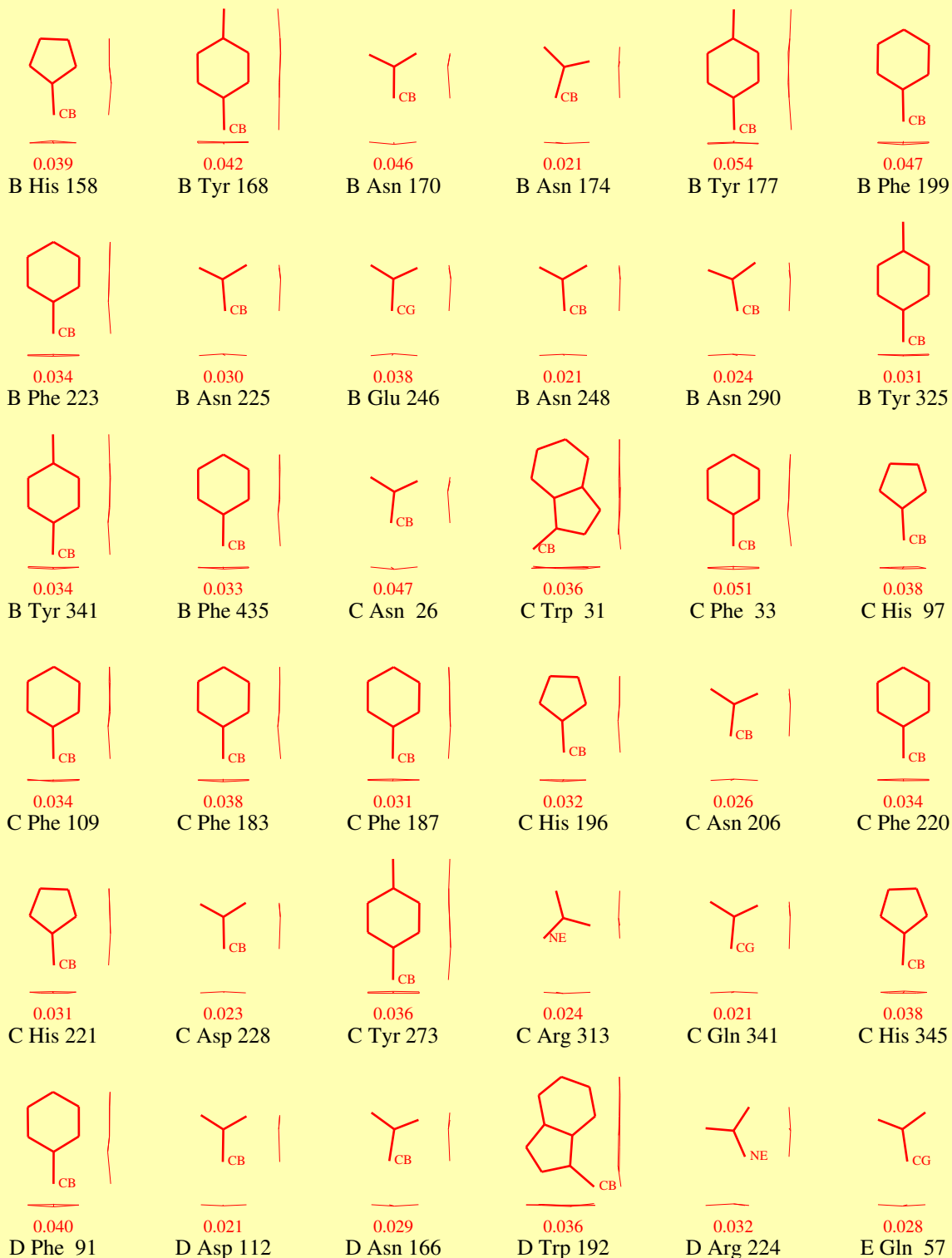
Bond angles differing by > 10.0 degrees from small-molec values. Values shown: "ideal", actual, diff.

### Planar groups



# Distorted geometry pdb1sqv

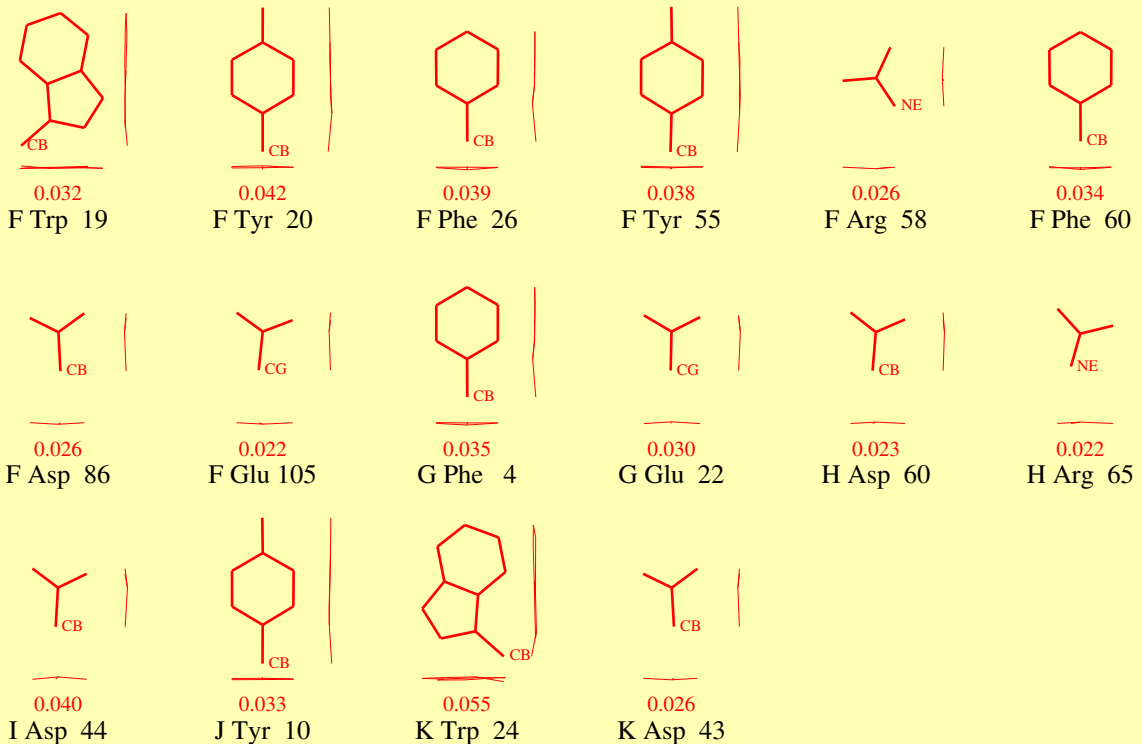
## Planar groups (contd)



# Distorted geometry

## pdb1sqv

### Planar groups (contd)



Sidechains with RMS dist. from planarity > 0.03A for rings, or > 0.02A otherwise. Value shown is RMS dist.